MECHANISTIC INVESTIGATION OF REARRANGEMENT OF AMMONIUM YLIDES

A Dissertation

by

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ABSTRACT

A central aim of physical organic chemistry is the elucidation of reaction mechanisms. This knowledge is then usable in the rational control of reactions and the development of new synthetic methodology. A reaction mechanism is generally viewed as consisting of the sequence of intermediates and transition states connecting starting material and products, and it would be expected that any experimental observation can be understood from the mechanism. In this way, the applicability of transition state theory (TST) is an implicit assumption in the description of reaction mechanisms and particularly the understanding of rates and selectivity. However, TST sometimes fails to account for experimental outcomes. The main goal of this dissertation is to investigate mechanisms of reactions where ideas outside of TST are needed to explain observations.

The origin of competing [2,3]- and [1,2]-rearrangements of ammonium-ylides was studied. The [2,3]-rearrangement is an allowed concerted pericyclic reaction while the [1,2]-rearrangement is forbidden and should occur by a stepwise process. The mechanism was investigated by a combination of experiments, standard theoretical calculations and dynamic trajectory calculations. The experiments include the measurement of kinetic isotope effects (KIEs), crossover experiments and temperature dependence of product ratio. The theoretical calculations predict an early and loose transition state for [2,3]-rearrangements. The theoretically predicted KIEs are in good agreement with experimental KIEs. Dynamic trajectories from an early and loose [2,3]-transition state showed that from a single transition state there is a bifurcation on the free

energy surface. One of the paths is concerted that leads to [2,3]-rearrangment product. However, an alternative path involving cleavage leads to diradicals that can recombine to give both [1,2]- and [2,3]-products. This partitioning of dynamic trajectories was supported by the crossover experiment because the [2,3]-product showed less crossover compared to the [1,2]-product. Although the concerted path has an enthalpic advantage over the cleavage path, the cleavage path has an entropic advantage. This is supported by the fact that higher temperatures favored [1,2]-product.

Since the competition of concerted [2,3]-rearrangement and bond cleavage observed experimentally is accounted for by the outcome of trajectories passing through the formal [2,3]-rearrangement transition state, we suggest here that the cleavage is facilitated by the pericyclic stabilization of the [2,3]-rearrangement transition state. Overall, we here propose that the common competition between the [2,3]- and [1,2]-rearrangement arises due to this dynamic effect.

Dynamic trajectories from the formal [2,3]-rearrangement transition state leads to cleavage because the transitions state is early and loose. Stabilization of the ylides through hydrogen bonding shifts the transition state later. Therefore, the introduction of hydrogen bonding disfavors the cleavage from the formal [2,3]-transition state. This allowed us to control the competition.

DEDICATION

TO MY FAMILY AND RATHINDRANATH MUKHERJEE

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NOMENCLATURE

KIE(s)	Kinetic Isotope Effect(s)
TS	Transition State
TST	Transition State Theory
VTS	Variational Transition State
VTST	Variational Transition State Theory
DMSO	Dimethyl sulfoxides
DCM	Dichloromethane

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CHAPTER I

INTRODUCTION

General Overview

Our daily life is closely dependent on the progress of chemical science. The contribution of chemistry to society depends chiefly on synthetic chemistry. Synthesis is challenging. One of the oldest but most difficult challenges synthetic chemists face is the avoidance of side products in reactions. Side products are a waste of materials and interfere with the purification of the desired molecules. Separations can be particularly difficult when the side product is isomeric with the desired target molecule. The rational avoidance of side products requires an understanding of the underlying mechanism involved in the chemical process. This is one reason that the elucidation of organic reaction mechanisms is a central goal of physical organic chemistry.

The conventional methods for the study of reaction mechanisms are experimental, e.g. kinetic studies, substitution effects, solvent effects, isotope labeling, the observation or trapping of intermediates and crossover experiments.[1-13] However, experimental mechanistic chemistry has its limitations. In particular, experiments often fail to probe complex reaction processes and often only provide qualitative information about a reaction mechanism.[14] The advancement of computational chemistry in combination with statistical rate theories such as transition state theory (TST) has allowed chemists to theoretically approach the elucidation of reaction mechanisms and the prediction of reactivities and selectivities of organic reactions.[15,16] However,

theoretical studies often fail to account for the experimental observations. [17] Such failures can be the result of inaccuracies in the computational methods used to predict the energy surfaces. They can also be the result of approximations made in going from the potential energy surfaces provided by calculations to the prediction of experimental observations. This latter idea will be discussed in more detail later in the chapter. The separate limitations of experiments and theory can often be overcome by studies that combine experimental and computational techniques to approach the understanding of reaction mechanisms.

TST is the central statistical model to understand the rates and selectivities of chemical reactions. A transition state is often thought of a particular geometry that must be passed through in order to get from reactants to products, but more formally a transition state is a multi-dimensional surface that separates reactants from products. In TST, it is assumed that the rate of passage through the transition state is governed by the relative free energy of the transition state versus reactants at thermal equilibrium. According to TST, the product ratio in a chemical reaction depends on the difference in the free energies of differing transition states (TSs) leading to the competitively formed products. This understanding of product ratios is based on the implicit assumptions that the separate paths are taken by the starting material to each of the products. TST has been highly successful at rationalizing reactivities and selectivities, it has limitations. In particular, there are experimental observations that cannot be accurately predicted by TST.[18] We describe those observations as dynamic effects; the idea is that when TST

fails one must fall back on the more primitive but more complex consideration of the positions and momenta of atoms, i.e. their dynamics.

Dynamic Effects

In our research group, a primary aim is to identify and understand the reactions where TST fails to account for experimental outcomes.[19] The central topic of this dissertation is the understanding of the formation of more than one product in a class of reactions. We find that the dynamic effects are responsible for this outcome. A growing number of simple reactions have been found to exhibit dynamic effects, and a series of types of dynamic effects have been recognized.

An early example of a dynamic effect in organic chemistry involves the unusual stereochemistry of the rearrangement of vinylcyclopropane to cyclopentene. Extensive efforts to rationalize the stereochemical outcome based on TST failed. However, Doubleday found that a consideration of the trajectories associated with the rearrangement TS could account for the unusual stereochemistry.[20,21] In the mid-nineteen eighties, Carpenter suggested that dynamic effects could explain some unusual observations in a series of reactions.[22] The kind of dynamic effect recognized by Carpenter may be termed 'dynamic matching'. TST assumes that the energy in TS is statistically distributed for multistep mechanism. This requires that intramolecular energy redistribution (IVR) is faster than overcoming the barriers for subsequent reactions. In Carpenter's case IVR is not only slow but also the selection of subsequent TSs is the result of their energy being in specific modes that favor those TSs over

alternatives

Another, interrelated form of dynamic effect is non-statistical recrossing. In non-statistical recrossing the continuation of motion through initial TS leads to potential energy wall that reflects trajectories back over the initial TS. This form of recrossing is referred to as non-statistical recrossing because it is not predictable from statistical rate theories even when those rate theories have been modified to allow for recrossing. An example is variational transition state theory (VTST) in which the TS hyper surface is placed in such a way to minimize the effect of recrossing. In a case of recrossing that results from a reflection from a potential energy (PE) surface wall the VTST still does not satisfactorily allow for the amount of recrossing. This form of dynamic effect is interrelated because it again relies on IVR being relatively slow and in this case is simply slower than the motion along the reaction coordinate (RC).

Ussing and Singleton first experimentally showed non-statistical recrossing in the cycloaddition of cyclopentadiene with diphenylketene (Figure 1-1).[23]

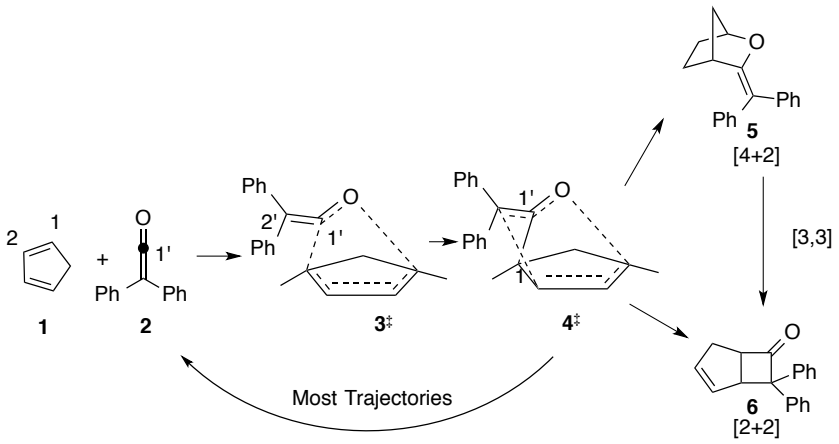


Figure 1-1. Cycloaddition of cyclopentadiene and diphenylketene

The initial process of the mechanism involves the formation of a bond between C1 and C1′. Trajectories pass through **3**‡ and C-C bond formation continues to afford geometries in the area of **4**‡. The saddle point **4**‡ is the TS of interconversion between [4+2]-product **5** and [2+2]-product **6**. Ussing and Singleton explained their experimental KIEs based on an unusual feature observed in dynamic trajectories. Trajectories that pass from **3**‡ into the area of **4**‡ tended to complete C-C bond formation but then recoil back across **3**‡ to afford either of the products **5** or **6**. C1 and C1′ bond formation has to be accompanied by a second bond formation. The second bond formation only has limited time to occur when the C1 and C1′ are close. If the second bond formation does not happen immediately the trajectory reverts to the starting material. Because the KIEs are determined in the region **4**‡ and not in the expected region **3**‡ experimental KIEs in this reaction could not be explained by TST.

A third form of dynamic effect results from what is referred to as “bifurcating

energy surfaces".[23] As discussed previously the formation of separate products from the same starting material is implicitly assumed in TST to result from separate TSs. The relative ratio of the product depends on the energy difference between the competing TSs. There are many instances where the predictions of ratio are unachievable because only one TS could be located. On a bifurcating energy surface this single TS could give rise to two or more products. Figure 1-2 shows two kinds of bifurcating potential energy surfaces. In the case of Fig.1-2 a), the potential energy surface is symmetrical and the minimum-energy path (MEP) bifurcates at a second transition state leading to two equivalent products. In case of 1-2 b), the surface is unsymmetrical and the MEP could connects the starting material to a single product. Trajectories however can lead to the second product. Since there is no TS associated with partitioning of trajectories between the two products TST cannot make any prediction on the product ratio.

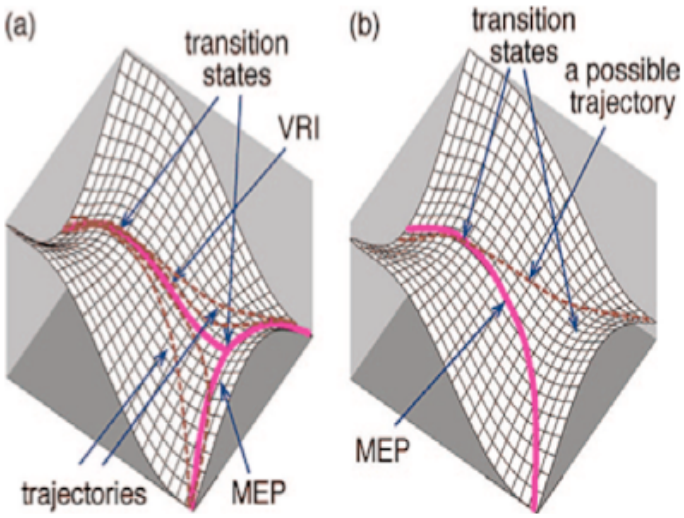


Figure 1-2. Symmetrical and unsymmetrical potential energy surfaces. a) Symmetrical potential energy surface (PES), which results in a bifurcating minimum energy path (MEP), leading to one product from the same transition state. b) Unsymmetrical PES leading to two non-equivalent products that are not in MEP

A seminal work by Oyola and Singleton used dynamic effects to explain the product selectivity in the hydroboration of alkenes.[19] Hydroboration of terminal alkenes followed by oxidation produces a mixture of primary and secondary alcohols. However TST predicts that amount of secondary alcohol should be negligible. In their work they successfully explained the origin of secondary alcohol. This is due to the fact that an intermediate π-complex reacts faster than their thermal equlibration.

In a similar study Quijano and Singleton found that the product selectivity of ozonolysis of vinyl ethers could only be explained if IVR is slower than the rate of the reaction.[24]

An example is the observation of Newtonian KIEs by Kelly and Singleton. [25]

Ordinary KIEs results from quantum mechanical effects associated with zero point energy (ZPE) and or tunneling. Kelly and Singleton observed isotope effects that were the results of selectivity on the downhill slope of a bifurcating surface in the dimerization of cyclopentadiene. This selectivity arises due to classical motion of the atoms, and the effect of ZPE is negligible.

A new type of dynamic effect referred to as entropic bifurcation is the central focus of this dissertation. In this class of dynamic effect there is no bifurcation on the potential energy surface. As a result downhill in potential energy surface leads to single product. However in the free energy there is a bifurcation that allows formation of more than one product. Since there is no bifurcation in potential energy surface the bifurcation in free energy surface arises due to the influence of entropy. In 2003 Yamataka, Aida and Dupuis saw a possible example of this kind of dynamic effect in their theoretical work on the rearrangement of $Me_3C\text{-}CHMe\text{-}OH_2^{+}$.[26] In that work the minimum energy path gives rise to a concerted loss of the leaving group and rearrangement. However many trajectories involves the loss of the leaving group without the second part of the process, rearrangement of the alkyl group. In 2005 Ussing and Singleton provided evidence for dynamic effect of this type in the solvolysis of aryldiazonium ion in water. In that reaction the loss of the leaving group is accompanied by the approach of water molecules and displacement appears to be a concerted substitution on the potential energy surface. However, water molecules are so loosely associated with the carbocation at the TS that entropy can favor their separation from the carbocation center. This allows the formation of long lived carbocation, despite the fact that it is always downhill on the

potential energy surface for the water molecules to approach the carbocation. Ussing and Singleton's work first demonstrates the experimental consequence of this dynamic effect.

This work on sigmatropic rearrangement in this dissertation arose from unusual observations in the literatures as will be discussed in the later chapter. The [2,3]-sigmatropic rearrangement routinely occur in competition with [1,2]-sigmatropic rearrangement.[27] This often limits the synthetic utility of the [2,3]-rearrangement. the [2,3]-rearrangement is an allowed concerted pericyclic reaction while the concerted [1,2]-rearrangement with retention is forbidden and as aresult it should occur by a stepwise mechanism.[27] This common competition between allowed [2,3] and forbidden [1,2] re arrangement intrigued us. We sought to investigate the origin of competition by combination of experimental studies and theoretical calculations. The experimental studies include the measurement of ^{13}C KIEs, observation of temperature dependence on product distribution and crossover experiments. It will be seen that TST cannot account for our observations and we envisioned that dynamic effects were important these reactions. In CHAPTER III and CHAPTER IV the mechanistic investigation will be described in detail.

Kinetic Isotope Effects

Isotopic substitution does not have any appreciable effect on the structure of a molecule, as the potential energy surface is independent of mass of the atom. Isotopologues generally follow the same reaction mechanism. However isotopes affect

the rate of a reaction. The difference in rate due to isotopic substitution is referred to as a kinetic isotopic effect (KIE). KIEs are one of the most useful probes of reaction mechanisms.[28] If an atom is directly involved in a bond making or breaking process in the rate-limiting step, the substitution by another isotope of the atom will lead to large change in rate of the reaction. This is called a primary KIE.[17,29] If the substituted atom is near the atoms involved undergoing bonding changes in the rate-limiting step, the effect on rate due to isotopic substitution is small. This is called a secondary KIE.[30] However, if the substituted atom is away from the atoms involved in bonding changes in the rate-limiting step, the effect of isotopic substitution is likely to be negligible. Thus KIEs provide information about the bonding changes in the rate-limiting step of a reaction.

According to classical mechanics, the frequency (υ) of a bond vibration depends on the mass and force constant (k) of the bond. The force constant depends on the strength of the bond. If two atoms having mass m_1 and m_2 are attached, the frequency of the bond will be [equation (1-1)] within the harmonic approximation.

$$\upsilon = (1/2\pi)*(k/m_r)^{1/2} \quad \text{where, } m_r = m_1m_2/(m_1+m_2) \qquad (1\text{-}1)$$

If one of the atoms is replaced by a heavier isotope, the reduced mass (m_r) will decrease which in turn will decrease the zero point energy (ZPE) as ZPE = 0.5*hυ, where h is Plank's Constant. For simplicity we will consider a particular case (Fig. 1-3), when hydrogen (H) of a C-H bond is replaced by deuterium (D). The zero-point energy will decrease D is heavier than H. Commonly, the force constants are smaller at the

transition state than they are in the starting material. Therefore, ΔE_D should be greater than ΔE_H (Figure 1-3). In this common case the lighter isotope will react faster. This order of reactivity is termed a normal KIE (Figure 1-3). However, there are cases where the force constants are larger at the transition state than they are in the starting material(s). In those cases, the heavier isotope will react faster. This is called an inverse KIE.

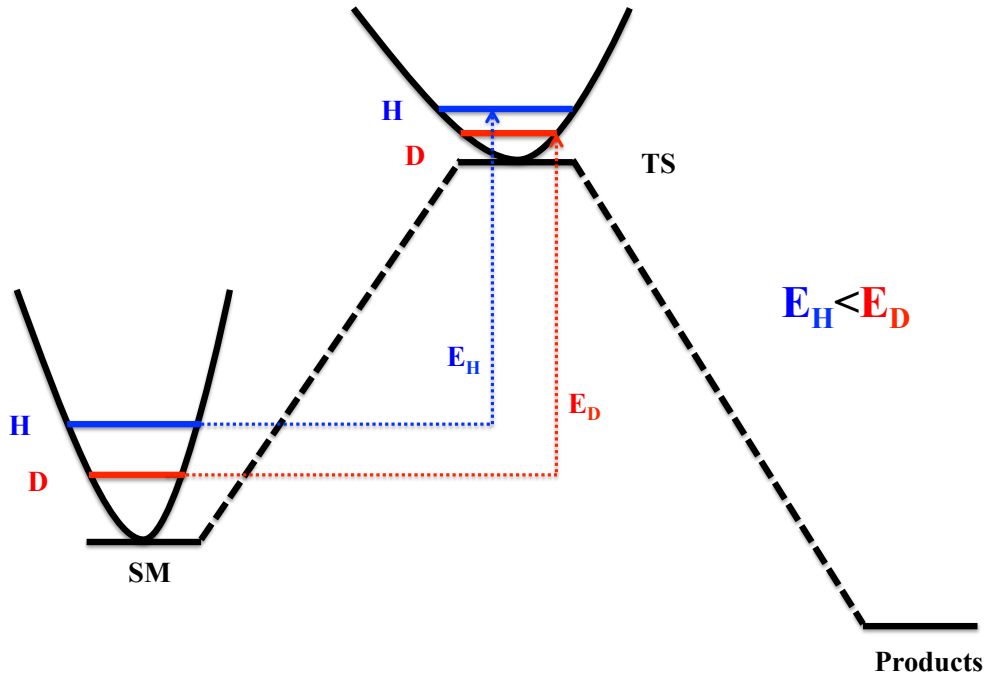


Figure 1-3. Origin of kinetic isotope effect

Traditionally, KIEs have been measured by synthesizing isotopically labeled molecules.[29] The synthesis of labeled molecules can be challenging. This makes many desirable KIE studies impractical. The measurement of KIEs at different positions in a molecule requires the synthesis of molecules labeled in different positions.[31]

In 1995 Singleton and Thomas developed a method to measure KIEs at natural abundance.[32] All of the KIEs reported in this dissertation were determined at natural abundance using the Singleton methodology. This method not only eliminates synthetic problems associated with the synthesis of isotopically labeled molecules, but also allows determination of KIEs at different positions. The methodology takes the advantage of the competition reaction that is inherent between isotopologues at their natural abundances.

As a reaction proceeds the unreacted staring material is enriched with slower reacting isotopomers and the product is enriched with faster reacting isotopomers. Accurate measurement of the changes in isotopic composition allows the calculation of the KIEs.

These measurements may be made on the starting material. A reaction is taken to high conversion (e.g. >80%). The unreacted starting material is then recovered from the reaction. The unreacted starting material in a reaction will be enriched with the slower reacting isotopes. NMR measurements under special conditions then allow us to compare the isotopic composition with material that was not subjected to the reaction. The relative isotopic composition (R/R_0) at each position in the molecule can be determined by the integrations of the peaks of the NMRs for the recovered material and

the non-reacted starting material. The KIEs can then be calculated from (R/R_0) and the conversion (*F*) using the following equation.

$$KIE_{SM(intermolecular)} = \log(1-F)/\log[(1-F)*(R/R_0)] \quad (1\text{-}2)$$

In many cases the recovery of staring material is too complicated. In these cases one can, measure KIEs based on NMR analysis of the product. In order to measure KIEs using the product, the reaction is taken to low conversion (e.g. <20%). The product is then isolated from the reaction mixture. In this case, the product will be enriched in faster reacting isotopomers. Another reaction is taken to 100% conversion. Since the conversion is quantitative the product would have the same isotopic composition present in the original starting material. The KIEs can be measured by integration of the NMR peaks as explained before. The equation is used to calculate the KIEs as follows.

$$KIE_{Product(intermolecular)} = \log(1-F)/\log(1-F*R/R_0) \quad (1\text{-}3)$$

Intramolecular KIEs measure the relative rate of reactions in positions that are equivalent in the starting material except for isotopic composition, but not in the product. The intramolecular KIEs provides information about the first irreversible step desymmetrizing the startin material, referred as the product-determining step. Intramolecular KIEs measure relative isotopic abundance between two atoms in a single molecule and do not need any measurement for a standard. Suppose there are two

carbons **a** and **b** which are equivalent in the starting material but not in the product. If ^{13}C abundance in the product at **a** is R_a and at b is R_b the intramolecular KIE at **a** is as follows.

$$KIE_{intra} = R_b/R_a \quad (1\text{-}4)$$

In 1947 Bigeleisen and Mayer proposed a theoretical model to predict KIEs quantitatively.[33] The equation is as follows.

$$KIE_{TST} = [\nu_1^{\ddagger}*(s_2/s_1)*f_{GS}]/ [\nu_2^{\ddagger}*(s_2/s_1)*f_{TS}] \quad (1\text{-}5)$$

Where,

$$(s_2/s_1)*f_{GS} = {}_i\Pi^{3N-6}[\nu_{2i}/\nu_{1i}]*[(1-\exp(-u_{1i}))/(1-\exp(-u_{2i}))]*[\exp(u_{1i}/2) / \exp(u_{2i}/2)]$$

$$(s_2/s_1)*f_{TS} = {}_i\Pi^{3N-7}[\nu_{2i}/\nu_{1i}]*[(1-\exp(-u_{1i}))/(1-\exp(-u_{2i}))]*[\exp(u_{1i}/2) / \exp(u_{2i}/2)]$$

$$u_i = h*\nu_i/k*T$$

The equation has three parameters, the temperature (T), the frequency of the vibrational modes (ν_i) and the reduced isotopic partition function or the isotopic fractionation factor (f). Bigeleisen's equation relies on conventional TST and the harmonic approximation but it has been highly successful in predicting experimental

KIEs. Commonly, the equation fails to predict KIEs in hydrogen-transfer reactions, as significant tunneling is associated with hydrogen transfers.[33b]

Tunneling refers to the quantum mechanical phenomenon where a particle traverses through a barrier that it classically could not surmount. This phenomenon could be associated with any of the vibrational modes associated with a molecule. However, this multi dimensional allowance for tunneling in all vibrational modes is complicated, instead only the modes associated with the bond changing process are considered. The resulting one-dimensional tunneling correction is defined and applied to give a modified calculated, KIE_{calc}, as shown in the equation below.

$$KIE_{calc} = KIE_{TST} * KIE_{1D\text{-}corr} \quad (1\text{-}6)$$

Where,

$KIE_{1D\text{-}corr} = [u_1/2\sin(u_1^{\ddagger}/2)]/ [u_2/2\sin(u_2^{\ddagger}/2]$

CHAPTER II

DEVELOPMENT AND APPLICATIONS OF [2,3]-SIGMATROPIC REARRANGEMENT IN ORGANIC CHEMISTRY

Sigmatropic Rearrangement

Sigmatropic rearrangement is a special class of reaction where a σ-bond migrates to a new site within the molecule via a transient conjugated electron system. There are different types of sigmatropic rearrangements. For example, lets suppose that during a reaction one end of the σ-bond traverses a atoms and the other end traverses b atoms then the sigmatropic rearrangement would be termed as [a,b]-sigmatropic rearrangement. Considerable mechanistic studies have been carried out on sigmatropic rearrangements because of their synthetic utilities. These studies revealed that many sigmatropic rearrangements proceed via a concerted pathway.[34,35] However, there are sigmatropic rearrangements, which are not concerted and proceed via a stepwise mechanism involving diradicals or ion-pairs.[36,37] Due to the cyclic nature of the TS the concerted sigmatropic reactions follow the Woodward-Hoffmann pericyclic rule.[27,38] Even though stepwise sigmatropic rearrangements are often encountered, concentered sigmatropic rearrangements have predominately been used by synthetic chemists due to their high yield and stereospecificity.[39]

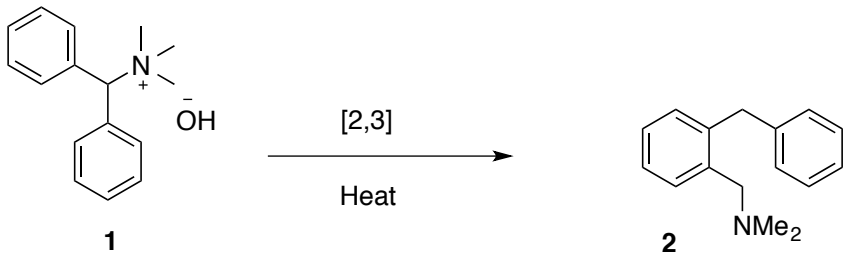
[2,3]-Sigmatropic Rearrangement

Among concerted pericyclic reactions, the [2,3]-sigmatropic rearrangement has drawn much attention due to its synthetic utilities.[40,41] This class of rearrangements has been observed, either in charged species or charge-separated species.

Since [2,3]-sigmatropic rearrangement is an allowed concerted pericyclic process it is often associated with high yield and high regio- and stereoselectivity. Due to these virtues, synthetic chemists often exploited [2,3]-sigmatropic rearrangement to achieve their synthetic goals.[39,42]

The history of [2,3]-sigmatropic rearrangement is dated back in 1937. When Sommelet evaporated aqueous solution of **1** in vacuum desiccator over phosphorus pentoxide under sunlight **2** was produced in modest yield. Similar result was obtained when **1** was heated to 145 °C.[43] That result indicated that sunlight merely provided the heat energy for the chemical transformation.

Scheme 2-1



1 **2**

However, in 1951 Hauser did the first detailed systematic study of base mediated rearrangement of benzyl quaternary ammonium salts.[44] In that work $NaNH_2$ was used as the base instead of hydroxide to deprotonate the ammonium salt to promote [2,3]-sigmatropic rearrangement. They also reported the synthesis a fully hexamethylbenzene by repeated use of [2,3]-sigmatropic rearrangement. The synthesis of hexamethylbenzene showed potential synthetic utility of [2,3]-sigmatropic rearrangement.

Over the years new classes of [2,3]-sigmatropic rearrangement have been discovered e.g. Wittig rearrangement, aza-Wittig rearrangement, thio-Wittig rearrangement and selenium based [2,3]- rearrangement etc.[45-48] Similar to the Sommelet Hauser rearrangement these reactions have also been used extensively for general methodology development and total synthesis of complex organic molecules.

Sommelet-Hauser Rearrangement

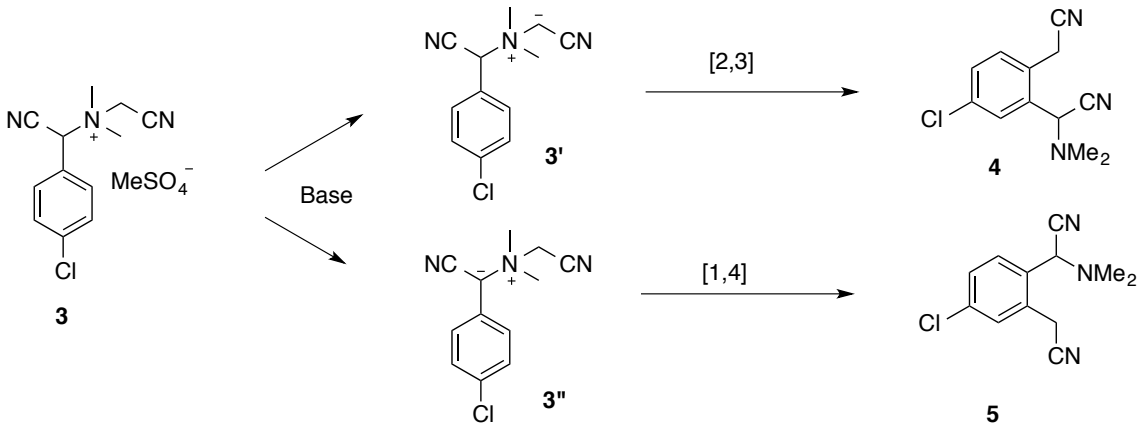
Since its inception, many researchers studied Sommelet-Hauser rearrangement. Ollis made considerable effort to understand the nature of the base mediated sigmatropic rearrangement of ammonium salts.[49-60] His experimental mechanistic studies unravel many characteristics of [2,3]-rearrangement. He explored the substitution and solvent effects on the product distribution when other competing rearrangements were competing. In his pioneering work on [2,3]-sigmatropic rearrangements of ammonioamidates, he reported the first experimental evidence of a case which may

follow a stepwise [2,3]- sigmatropic rearrangement that is otherwise considered to happen only in concerted way.[51]

Methods of Generation of Ylides

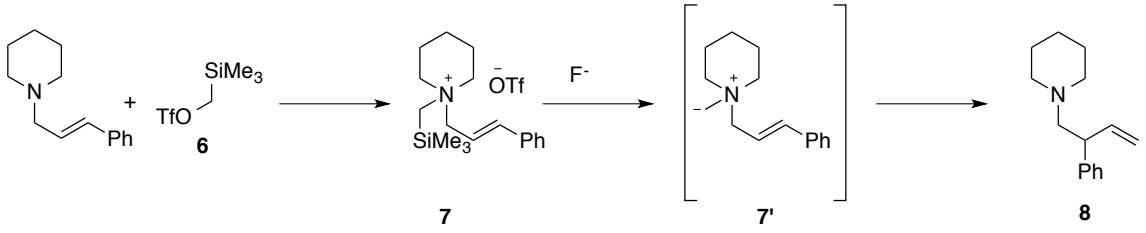
Even though initially the generations of ylides were predominately done by deprotonation of ammonium salts with suitable bases comparable acidity of different hydrogen atoms within a molecule led to regiochemical problems. For example, when **3** was treated with a suitable base the deprotonation occurs either at the benzylic position or at one of the methyl carbons leading to mixture of products.[61,62]

Scheme 2-2



In order to address this problem Vedejs developed a new method of formation of N-ylides that can undergo desired [2,3]-sigmatropic rearrangement (Scheme 2-3).[63]

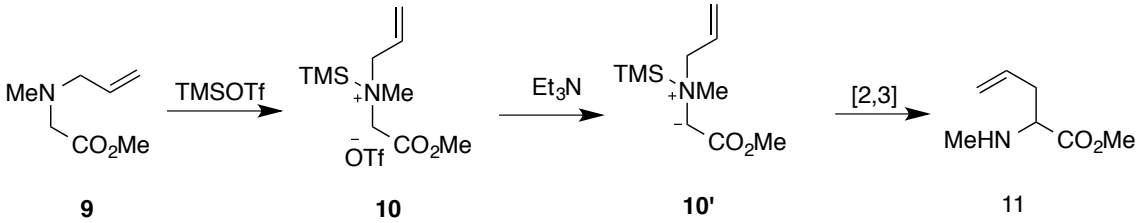
Scheme 2-3



In his work, he reacted a tertiary amine with **6**. The resulting ammonium salt **7** was then treated with CsF to generate ylide **7′**. The ylide, **7′** then undergo [2,3]-sigmatropic rearrangement smoothly to afford **8**. However, in this particular case traditional base mediated ylide generation would lead to regiochemical problems due to comparable acidity of different hydrogen atoms attached at different carbon centers. Later Sato extensively used this method of ylide generation for regioselective [2,3]-sigmatropic rearrangement. In his initial work, Sato limited his study towards the effect of substituents and solvents on the outcome of [2,3]-sigmatropic rearrangement.[35,64-74] However, in his later work he utilized [2,3]-rearrangement to achieve synthetic goals. He exploited [2,3]-sigmatropic rearrangement for regioselective ring enlargement of cyclic amines and for synthesis of spiro compounds.[75,76]

Another way of generating ylides was done by Nakai. Nakai developed Lewis acid mediated ylide formation (Scheme 2-4). He reacted **9** with TMSOTf to generate the ammonium salt **10**. The ammonium salt, **10** was then treated with triethylamine to afford ylide **10′**. The ylide **10′** then undergo [2,3]-rearrangement to afford **11**.[77]

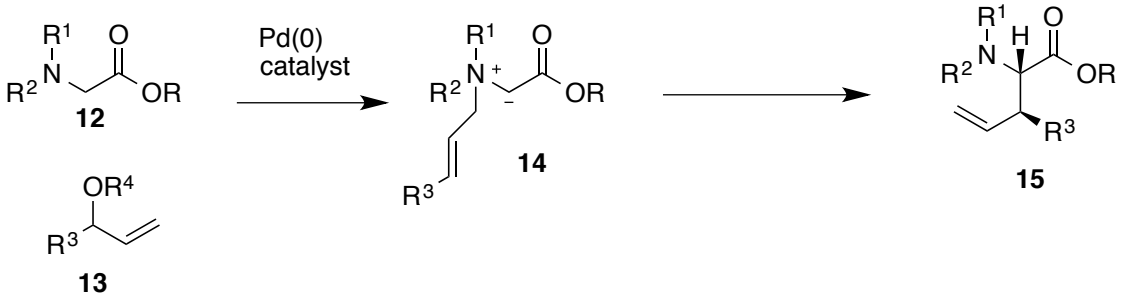
Scheme 2-4



9 **10** **10'** 11

Recently, Tamber group developed novel palladium catalyzed ylide generation. In his work he generated **14** by Pd-catalyzed reaction between **12** and **13**.[77,78] The ylide, **14** then undergo [2,3]-sigmatropic rearrangement to afford **15**.

Scheme 2-5



Diastereosectivity

[2,3]-sigmatropic rearrangements are expected to show high diastereoselectivity because this type of rearrangement is associated with cyclic TS. Depending on the

substituents present in the substrates up to two new stereogenic centers could be generated. The diastereoselectivity is found to be controlled by anion stabilizing groups (Z) and the conformational preference of the allylic moiety (Figure 2-1).[49,79]

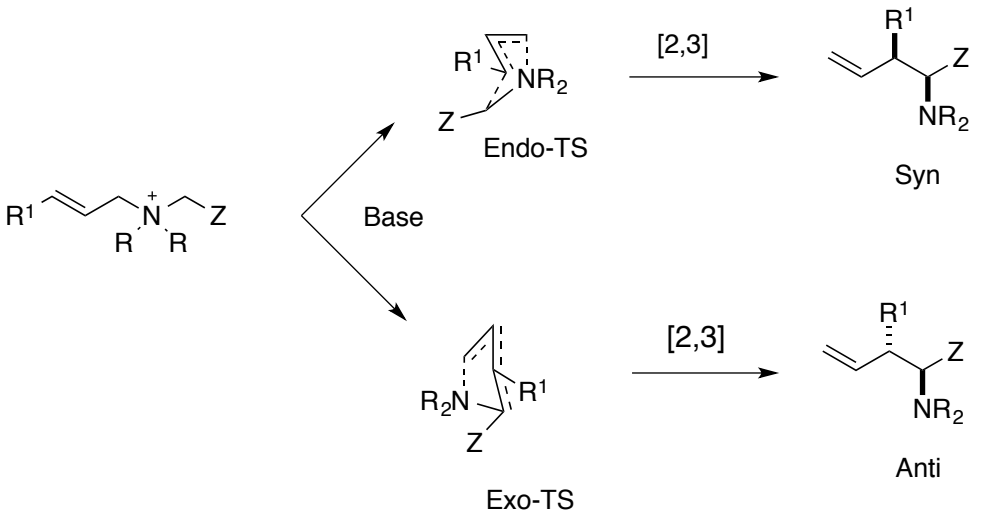


Figure 2-1. Diastereoselectivity by competing exo- and endo- TS

Even though conclusive rationale could not be drawn to explain the stereochemical outcomes, it is often found that in case of acyclic ylides having carbonyl, as the anion-stabilizing group the Exo-TS is favored over Endo-TS. However, in the case of alkynyl stabilizing group rearrangement proceeds preferentially via Endo-TS. It is important to mention that with the same anion-stabilizing group the Z-olefins exhibit opposite diastereoselectivity of the E-olefins. This observation indicates that the anion-stabilizing group plays a role in controlling the diastereoselectivity of the [2,3]-

rearrangement. However, often the diastereoselectivity is found to be low. This low diastereoselectivity indicates that in many cases the energy difference between the competing Exo- and Endo- TSs are small.

In contrast to the acyclic ylides cyclic ylides with carbonyls as the anion-stabilizing group have been found to prefer Endo-TS.

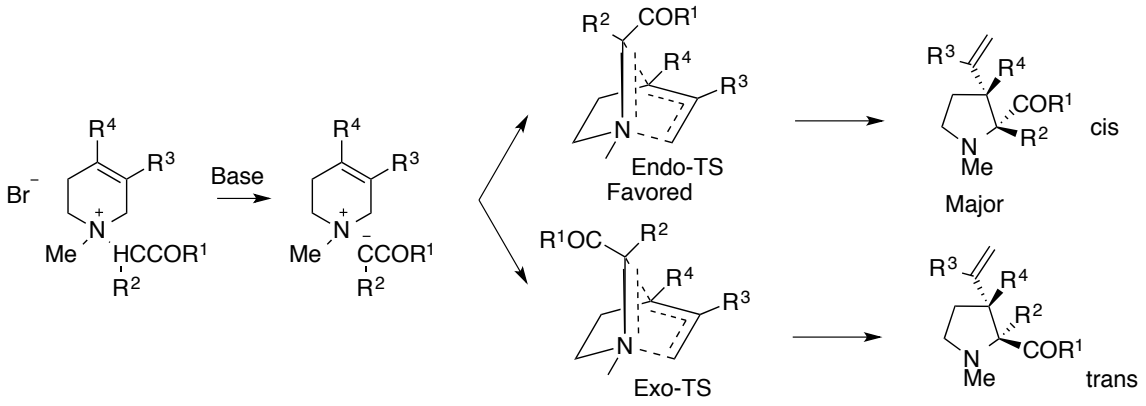


Figure 2-2. Reason of high diastereoselectivity of cyclic N-ylides

Ollis attributed this stereoselectivity to the secondary orbital interaction between the carbonyl moiety and the double bond.[14] In general the cyclic ylides tend to show higher selectivity compared to their acyclic analogues. This is perhaps due to the fact that cyclic systems are structurally more constrained compared to their acyclic counterparts leading to an increased energy difference between the competing Exo- and Endo-TS.

Besides the above-discussed stereosectivity [2,3]-sigmatropic rearrangement, in principle should exhibit another form of stereoselectivity, preferential geometry around the double bond. Predominately, [2,3]-sigmatropic rearranged products give E-isomer as the major product.[36] The origin of this selectivity is attributed to the fact that X prefers to occupy the equatorial position over the axial position at the TS to minimize the $A^{1,3}$-strain (Figure 2-3).

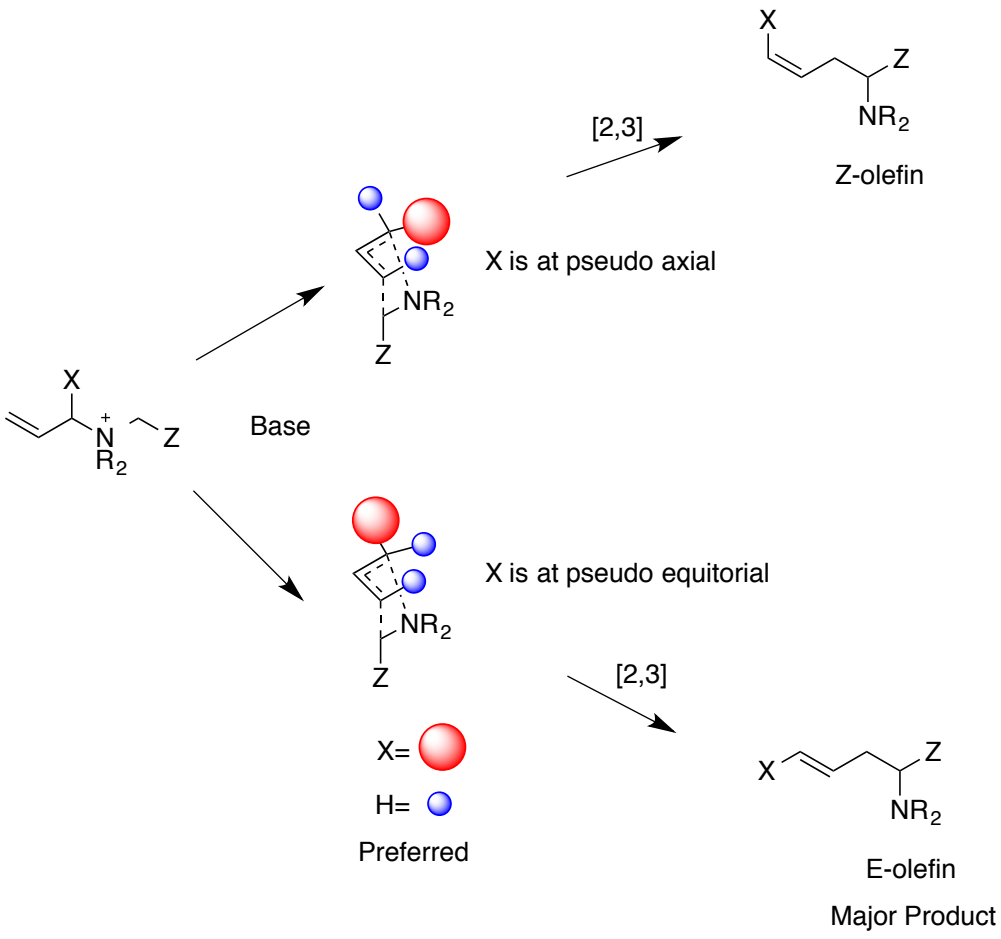
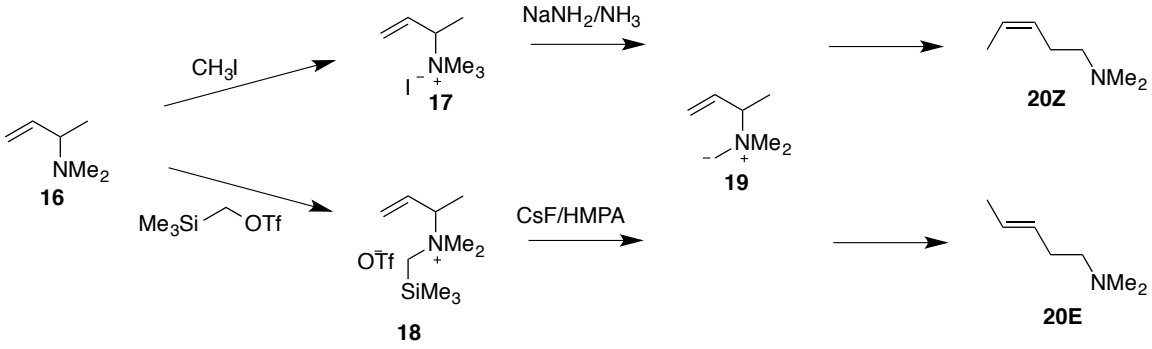


Figure 2-3. Diastereoselectivity of the newly formed double bond

Even though, commonly E-isomer is preferred over Z-isomer, Honda reported Z-selectivity.[80] Their work is particularly useful as they were able to obtain E- and Z-isomers selectively by changing the reaction conditions (Scheme 2-6).[81]

Scheme 2-6

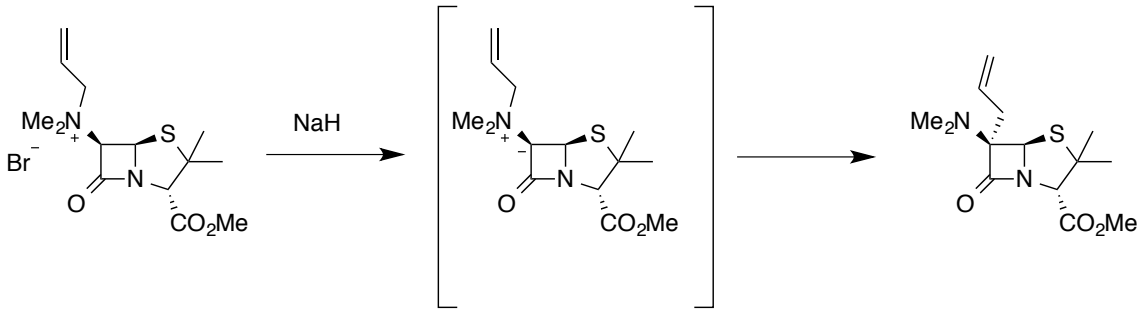


Asymmetric Synthesis

As [2,3]-sigmatropic rearrangement is an allowed pericyclic process it was envisioned by many researchers that this reaction could be employed to achieve asymmetric transformation.

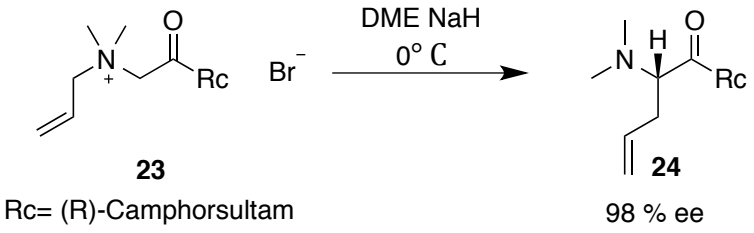
To our knowledge asymmetric [2,3]-rearrangement of ammonium ylides was first reported by Baldwin. He reported base-induced stereoelective [2,3]-sigmatropic rearrangement of allyl penicilium salt (Scheme 2-7).[82]

Scheme 2-7



Similarly, Trost group reported the first [2,3]-sigmatropic rearrangement on sulfonium ylides.[83] However, until recently asymmetric rearrangement of ammonium ylides was limited to cyclic systems. Sweeney was the first to report the asymmetric [2,3]-rearrangement of acyclic ammonium ylides (Scheme 2-8).[42,84] In that work, Oppolzer camphorsultam auxiliary was used to induce chirality during the rearrangement. Even though they were able to achieve very high enantiomeric excess their asymmetric induction was substrate control. This limited the scope of their work.

Scheme 2-8



Later Somfai addressed this problem by using chiral diazaborolidine as the Lewis acid to promote [2,3]-rearrangement.[39,85,86] Unlike, the previous case their asymmetric induction was reagent control allowing more substrate scope.

[2,3]-Wittig Rearrangement

It has been found that deprotonated allyl ethers undergo [2,3]-sigmatropic rearrangement. This rearrangement was termed as [2,3]-Wittig rearrangement.[87] This rearrangement was named after Prof. Wittig because he previously reported [1,2]-sigmatropic rearrangement of deprotonated benzylic ethers.[37,45] The following figure is showing the general scheme of [2,3]-Wittig rearrangement. The Z group is usually an electron-withdrawing group that stabilizes the negative charge at the adjacent carbon center of the anion.

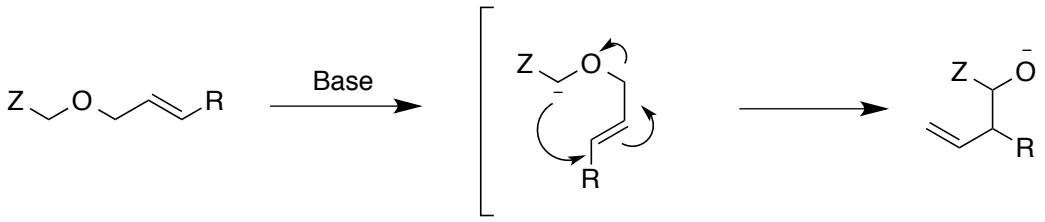
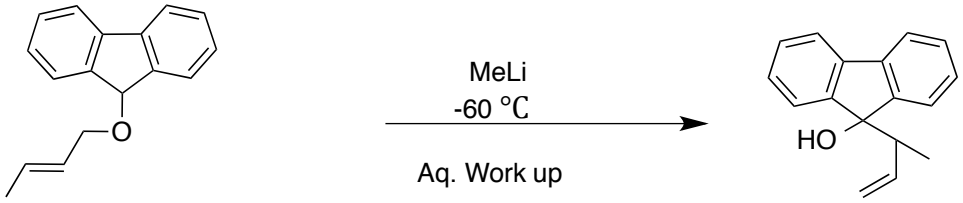


Figure 2-4. General scheme for [2,3]-Wittig rearrangement

Schöllkopf reported that allyl fluorenyl ether **25** smoothly undergoes [2,3]-rearrangment at -60 °C when reacted with MeLi.[87]

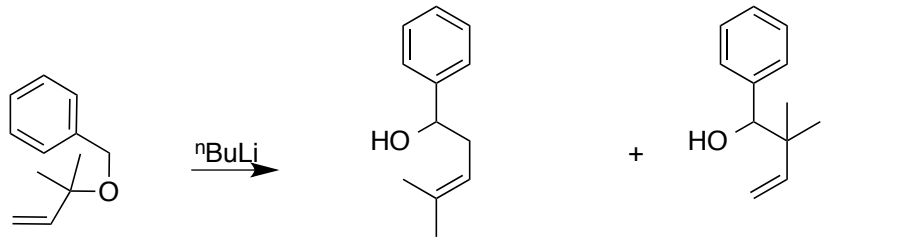
Scheme 2-9



25 **26**

Later, Rautenstrauch and Baldwin independently reported base mediated sigmatropic rearrngment of allyl ethers **27** and **29**.[88,89]

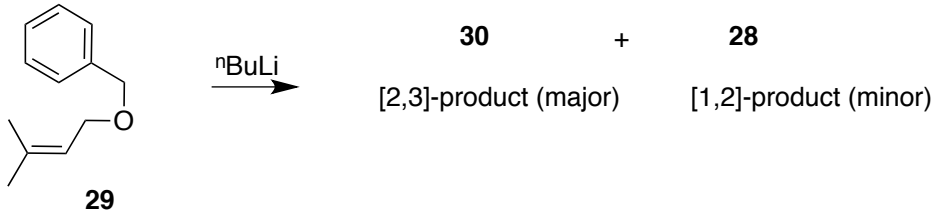
Scheme 2-10



27

28
[2,3]-product (major)

30
[1,2]-product (minor)



29

30 + **28**

[2,3]-product (major) [1,2]-product (minor)

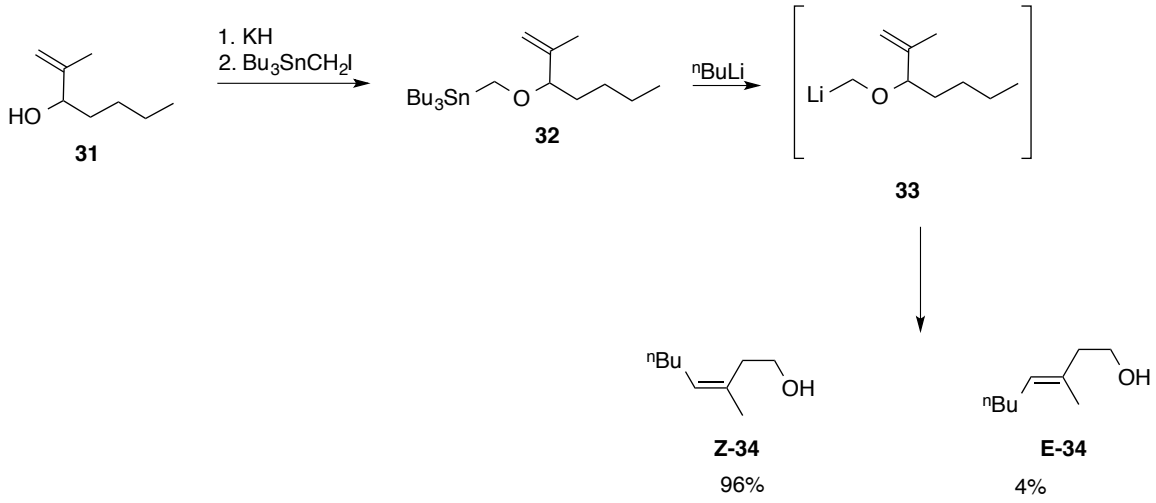
Both the research groups found that the [2,3]-rearrangements were competing with the [1,2]-rearrangements under the reaction conditions. This competion sometimes limits synthetic utilities of [2,3]-Wittig rearangement.[90] This competion will be discussed in detail in the later part of this chapter.

Diastereoselectivity

Similar to the [2,3]-rearrangment of ammonium ylides the newly formed double bonds predominately show E-selectivity.[45,89] The origin of E-selectivity is perhaps the same as in case the of the rearrangment ammonium ylides (Figure 2-3). However, it has been found that the substitutions at the allylic center reduces the stereoselectivity. This is likely due to the lowering of the energy difference between the competing Exo- and Endo- TSs affording different diastereomers.[41]

However, Still developed a method to prepare Z-double bond by [2,3]-Wittig rearrangment employing an organotin intermediate (Scheme 2-11). They deprotonated **31** with KH and then reacted the resulting alkoxide with iodomethyltributyltin to generate the allyl stannylmethyl ether **32**. After that they treated **32** with ^{n}BuLi at -78 °C to afford lithiated ether **33**. The lithiated ether under the reaction conditions underwent [2,3]-rearrangement to afford Z-34. Spectral analysis suggested that the ratio of **Z-34** to **E-34** was 96:4.[91]

Scheme 2-11



In order to rationalize the stereochemical outcome they qualitiatively examined the relative stability of the competing TSs, **TS-Z** and **TS-E** affording E- and Z-isomers respectively (Figure 2-5). Experimental result suggested that **TS-Z** should be of lower energy compared to **TS-E**. In order to rationalize this, they suggested that the steric interaction between pseudoequitorial ^{n}Bu group and methyl group in **TS-E** is more distabilising comapared to the interaction between pseudoaxial ^{n}Bu and pseudoequitorial methyl group in **TS-Z**. This can be understood the following way. The TS for the rearrangment should be very early as the carbanion center is not stabilised by any electronwithdrawing group. This early TS has stereochemical consequences.

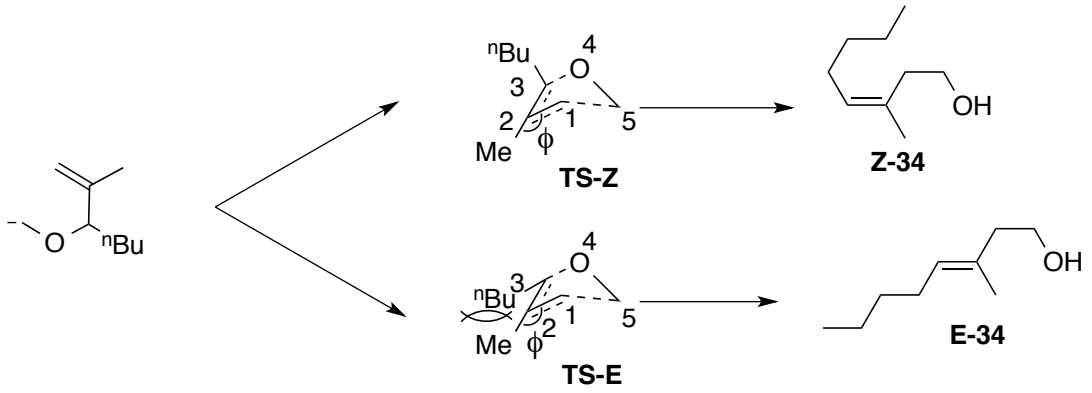


Figure 2-5. Mechanistic rationalization of Z-selectivity in Still-Wittig rearrangement

In **TS-Z** the angle (Φ) between the planes defined by C^1-C^2-C^3 and C^2-C^3-O^4 is greater than 90°. This in turn decreases the steric distabilization caused by pseudoaxial ^{n}Bu group. Secondly, in the alternative TS, **TS-E** the methyl group at C^2 and ^{n}Bu group at C^3 are almost eclipsed to each other leading to distabilisation due to steric interaction. This hypothesis was further supported by another observation. They observed that when hydrogen atom is attached at the C^2 instead of a methyl group the stereoselectivity of the rearrangement process decreased. This supports the origin of stereoselectivity comes from the steric interaction between substituents at C^2 and C^3.

[2,3]-Wittig rearrangment could potentially exhibit another kind of diastereoselectivity. Depending on the substituents present in the substrate, up to two new stereogenic centers could be formed by this rearrangment. It has been found that with alkynyl stabilising group Exo-TS is favoured over Endo-TS. This preference of Exo-TS over Endo-TS results the formation of threo-homoallylic alcohol, **37** from E-olefin, **35** and erythreo-homoallylic alcohol, **38** from Z-olefin **36**.[92,93]

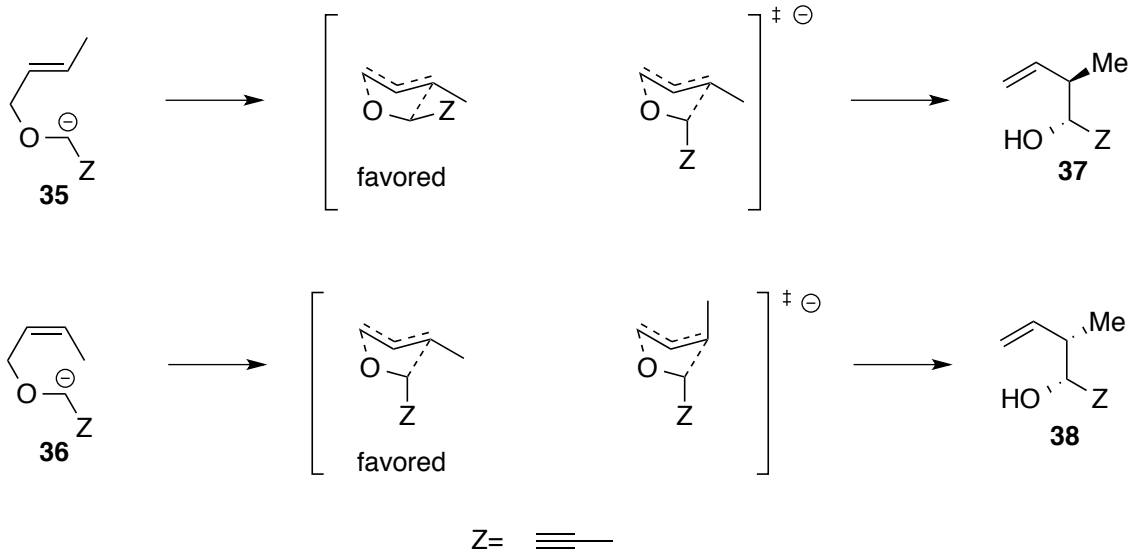


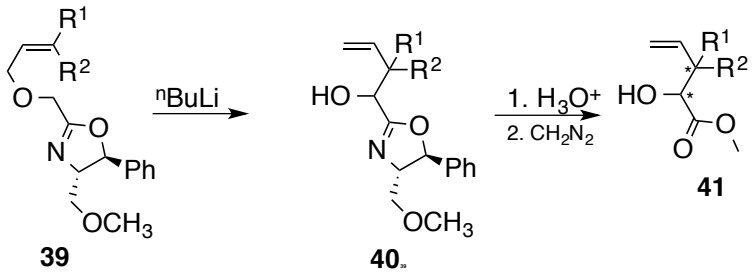
Figure 2-6. Double bond diastereoslectivity in [2,3]-Wittig rearrangement

Asymmetric [2,3]-Wittig Rearrangement

Due to the cyclic nature of the TS, [2,3]-sigmatropic rearrangement is expected to show high stereoselectivity. As a result [2,3]-Wittig rearrangement has been used to achieve asymmetric transformations. There have been many ways to achieve asymmetric transformation via [2,3]-Wittig rearrangement. Baldwin was the first to discover chirality transfer in [2,3]-Wittig rearrangement. In this class of asymmetric transformation, the starting material is enantioenriched and the original chiral center gets destroyed during the reaction but creates a new one in the product. Even though the product obtained via chirality transfer is optically active this kind of asymmetric transformation is of low synthetic utility since the original chiral center gets destroyed during the rearrangement. Alternative but more synthetically valuable approach is to use

a chiral auxiliary. The first reported asymmetric [2,3]- Wittig rearrangement was accomplished with Meyers' chiral 2-oxazoline ring (Scheme 2-12).[94]

Scheme 2-12



39 **40**

R^1=R^2=H, **R** (Major configuration)
R^1=CH_3, R^2=H, 2**R**,3**S** (Major configuration)
R^1=R^2=CH_3, **R** (Major configuration)

The chiral auxiliary was then removed via acidic workup. The exact reason of the stereochemical outcome is not known. However, it is suggested that **TSR** is favored over **TSS** as in **TSS** there is a steric interaction between the phenyl ring and the methyl of the crotyl group. This in turn favors the bottom face attack (Figure 2-7).

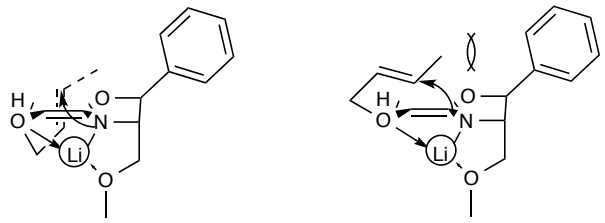


Figure 2-7. Chiral 2-oxazoline assisted asymmetric [2,3]-Wittig rearrangement. TSR is favored over TSS

This variety of asymmetric [2,3]-Wittig rearrangement is particularly useful for asymmetric synthesis of α-hydroxy acids. Detailed discussion of synthetic applications of [2,3]-rearrangement will be discussed in the next section of this chapter.

Aza-Wittig Rearrangement

Another kind of [2,3]-sigmatropic rearrangement is observed when tertiary allylic amines are treated with suitable bases.[95] This is a basically nitrogen-version of Wittig-rearrangement and is termed as aza-Wittig rearrangement. The general scheme of aza-Wittig rearrangement is shown in the Figure 2-8.

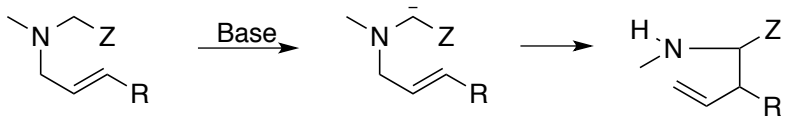


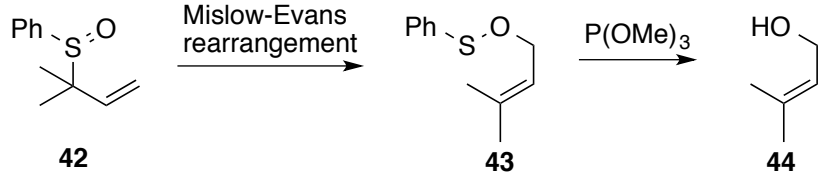
Figure 2-8. General scheme of [2,3]-aza-Wittig Rearrangement

However, unlike the case of Wittig rearrangement the literature reports on aza-Wittig rearrangement are rare and often this rearrangement process has been found to be sluggish.[96] This is probably due to lower stability of the carbanion since nitrogen is less electronegative than oxygen.

Mislow-Evans Rearrangement

Mislow and Evans discovered another class of [2,3]-sigmatropic rearrangement.[97] This rearrangement involves formation of sulfenate esters (**43**) from allyl sulfoxides (**42**) by [2,3]-sigmatropic rearrangement. The sulfenate esters (**43**) thus formed could be transformed to allylic alcohols (**44**) by thiophiles, organophosphites. This rearrangement is particularly useful to synthesize E-double bonds.

Scheme 2-13



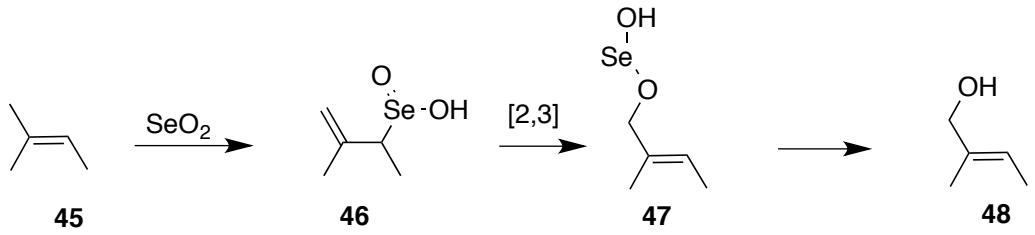
42 **43** **44**

Mislow-Evans rearrangement has been extensively used in total synthesis of many natural products. Detailed discussion of its application will be found in the later part of this chapter.

Selenic Acid Mediated Rearrangement

A related reaction to Mislow-Evans rearrangement is selenium oxide mediated oxidation of olefins to allylic alcohols. The mechanism of this reaction has been a mystery for years until Sharpless was able to explain the mechanism involving an initial ene-reaction followed by [2,3]-sigmatropic rearrangement.[98] Usually, the selenium (II) species (**47**), formed by rearrangement, decomposes to afford the allyl alcohol (**48**).

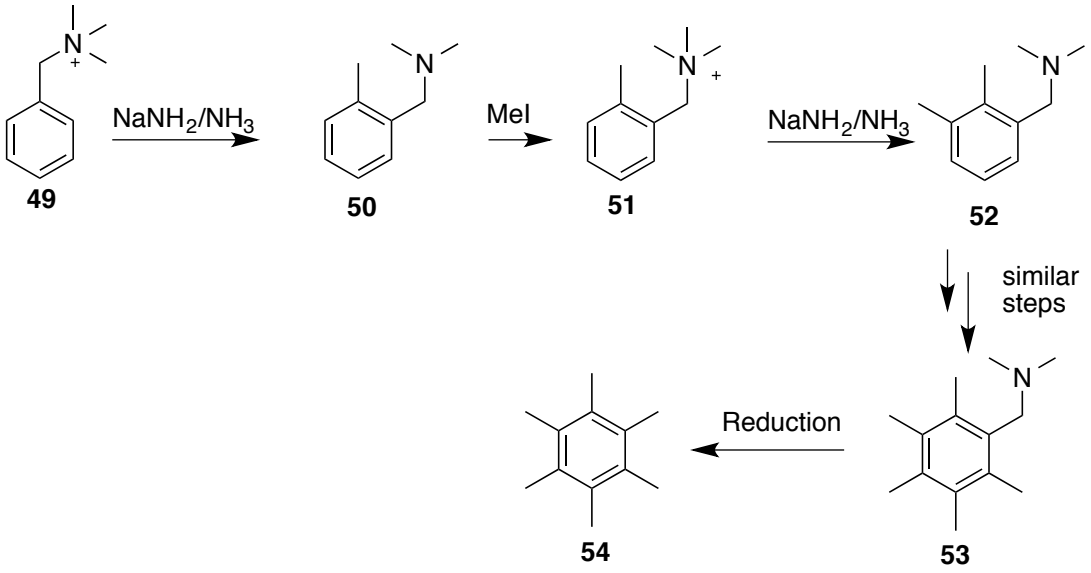
Scheme 2-14



Synthetic Application of [2,3]-Sigmatropic Rearrangement

For many years chemists used [2,3]-sigmatropic rearrangement to achieve their synthetic goals. Especially, [2,3]-rearrangement has been routinely employed to generate highly substituted carbon centers. Hauser, in his seminal work on [2,3]-rearrangement of ammonium ylides, was able to synthesize hexamethylbenzene, **54** from **49** by using [2,3]-sigmatropic rearrangement (Scheme 2-15).[44]

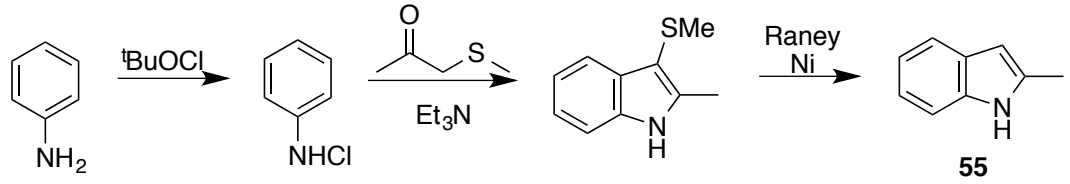
Scheme 2-15



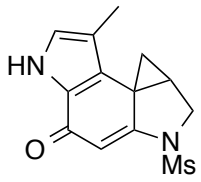
His initial work showed the potential of [2,3]-sigmatropic rearrangement in synthetic organic chemistry.

The synthetic utility of Sommelet Hauser rearrangement was recognized when Gassman utilized this particular reaction for one-pot synthesis of indoles (Scheme 2-16).[99]

Scheme 2-16



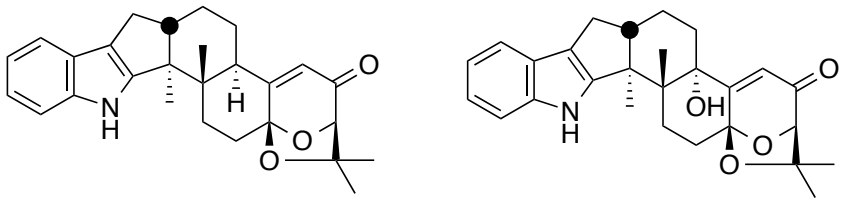
This reaction has particularly efficient compared to other synthetic methods for indole synthesis staring from anilines. However, in his original work he reported this particular synthetic method was unsuccessful when electron donating groups were present in the starting aniline. This problem was subsequently overcome by direct synthesis of aza-sulfonium salts. The aza-sulfonium salts were generated treating ketosulfides with bromine or chlorine followed by treatment with electron rich anilines. Then, those aza-sulfonium salts were treated with a suitable base to afford indoles. This particular modification was extremely useful for synthesizing 5- and 7-methoxyindoles natural products.[100] In 1981 Weirenga utilized modified Gassman indole synthesis to construct a part (Figure 2-9) of antitumor agent CC1065.[101]



56

Figure 2-9. Part of antitumor agent CC1065 synthesized by Weirenga

Also in 1992 Smith utilized Gassman indole synthesis for total synthesis of (+)-Paspalicine and (+)-Paspalinine (Figure 2-10).[102]

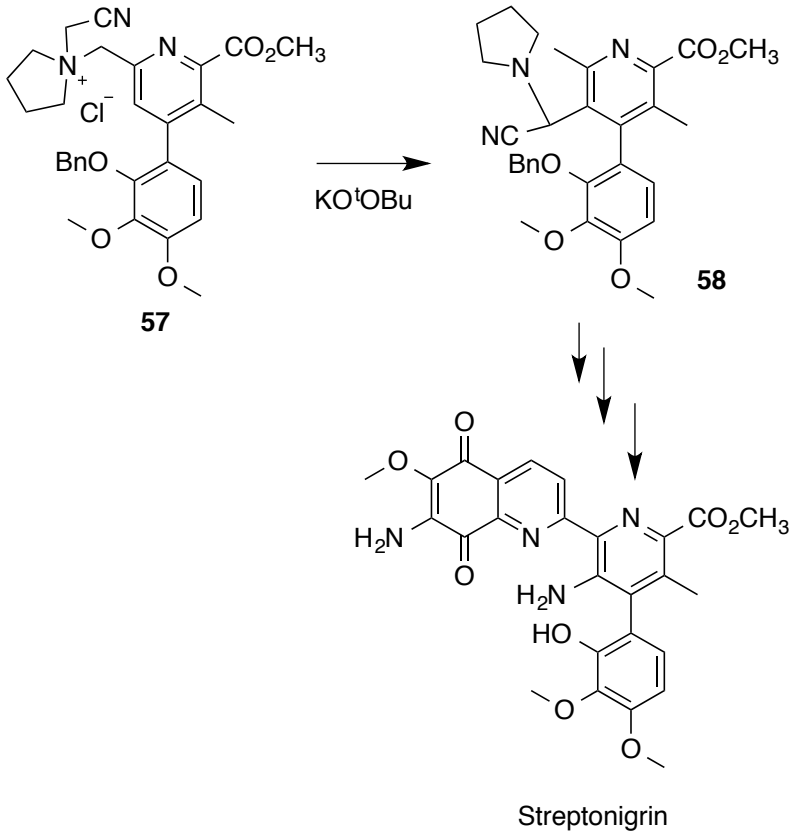


(+)-Paspalicine **(+)-Paspalinine**

Figure 2-10. Structures of (+)-paspalicine and (+)-paspalinine

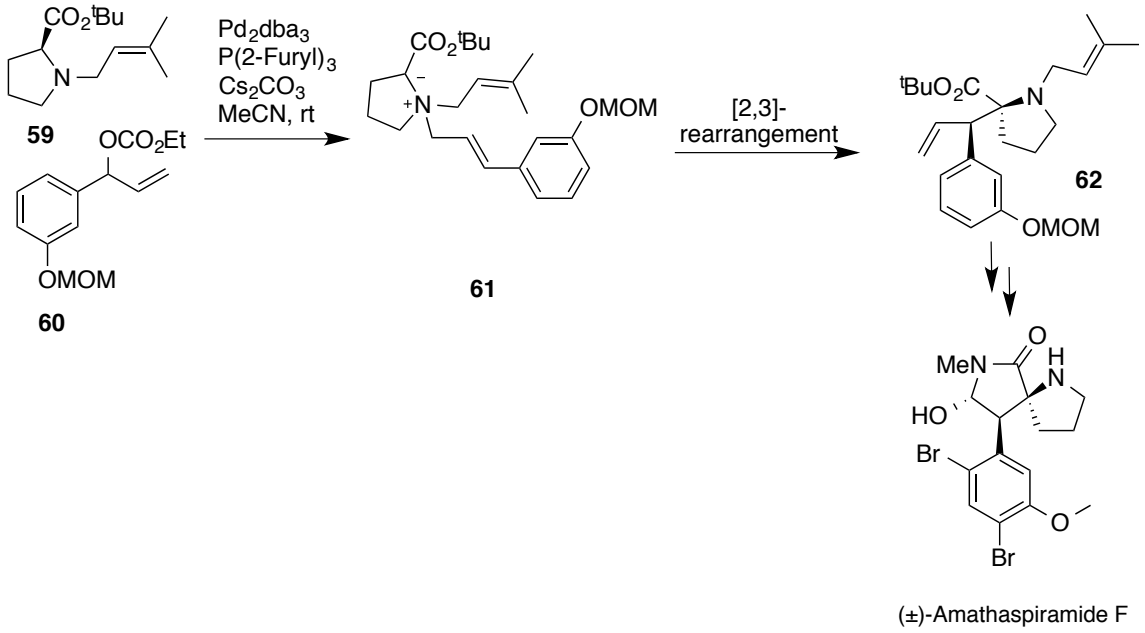
Weinreb used the Sommelet-Hauser rearrangement to transform **57** to **58** (Scheme 2-17). Further modification of 58 led to the desired natural product Streptonigrin.[103]

Scheme 2-17



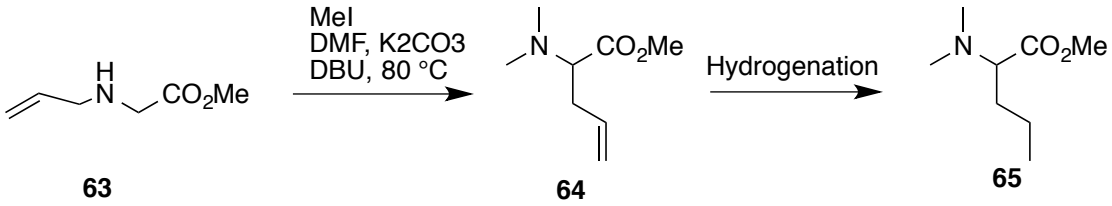
Recently, Tamber group utilized [2,3]-sigmatropic rearrangement of ammonium ylides during the synthesis of (±)-Amathaspiramide F (Scheme 2-18).[78]

Scheme 2-18



Besides total synthesis, Sommelet-Hauser rearrangement has been used extensively to synthesize non-proteogenic amino acids.[36,79] Especially it has been extensively used in the synthesis of non-proteogenic amino acids that are devoid of any α-hydrogen. Coldham, in his pioneering work was able to synthesize numerous amino acid derivatives in one-pot, via Sommelet-Hauser rearrangement (Scheme 2-19).[79]

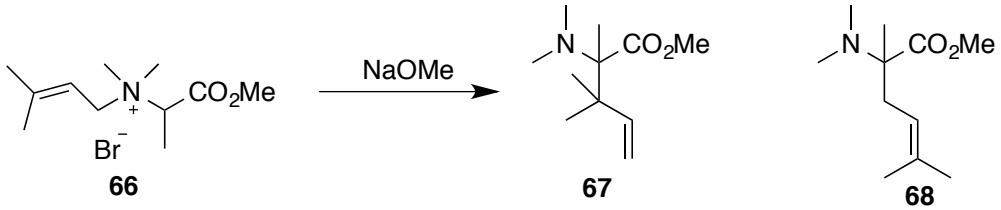
Scheme 2-19



Since in nature almost all amino acids exist in optically pure form asymmetric synthesis of non-proteogenic amino acids and their derivatives is important. Sweeny was first to report the asymmetric synthesis of unnatural amino acid derivatives via Sommelet-Hauser rearrangement using chiral auxiliary (Scheme 2-8).

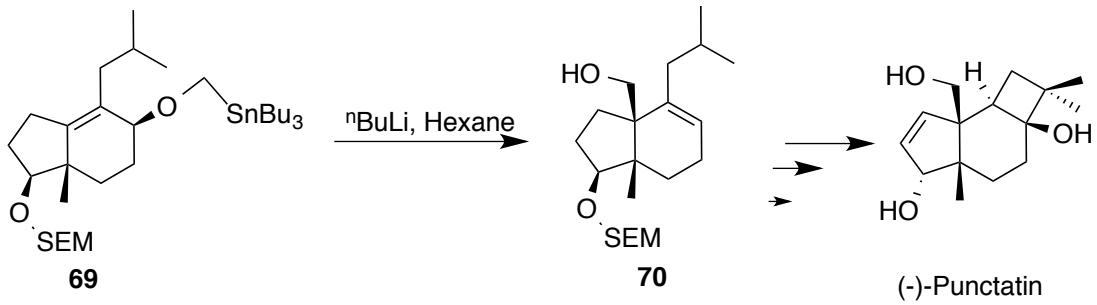
It has been reported that α-amino acid lacking α-hydrogen is involved in biosynthesis of antibiotics.[104] However, synthesis of quaternary α-center by conventional organic methods has always been challenging. Ollis was first to report the synthesis of a non-proteogenic α-amino acid derivative, lacking α-hydrogen via Sommelet-Hauser rearrangement.[36] However, his synthesis was complicated by competing [1,2]-rearrangement affording **68**.

Scheme 2-20



There are literature reports where [2,3]-Wittig rearrangement was employed to achieve total synthesis of natural products. In 1987 Paquette utilized this rearrangement at one of the key steps while synthesizing (-)-Punctatin A.[90] The enantioselective transformation of **70** from **69** was achieved by [2,3]-Wittig rearrangement.

Scheme 2-21



In addition, tandem [2,3]-Wittig rearrangement followed by Oxy-Cope rearrangement has been used for synthesis of brevicomine and oxocrinal (Figure 2-11).[105]

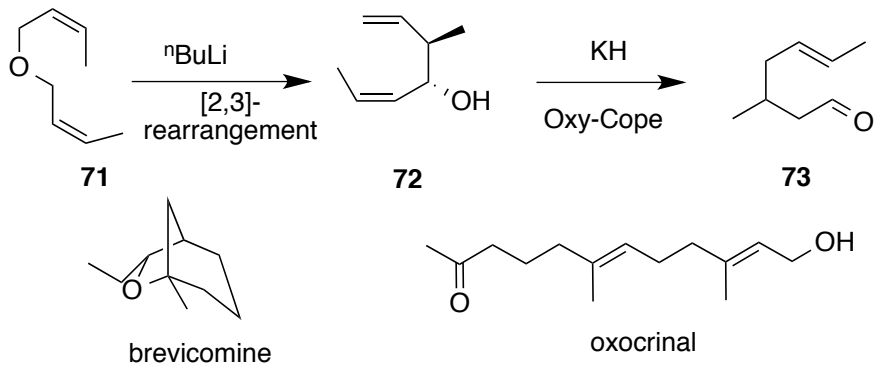
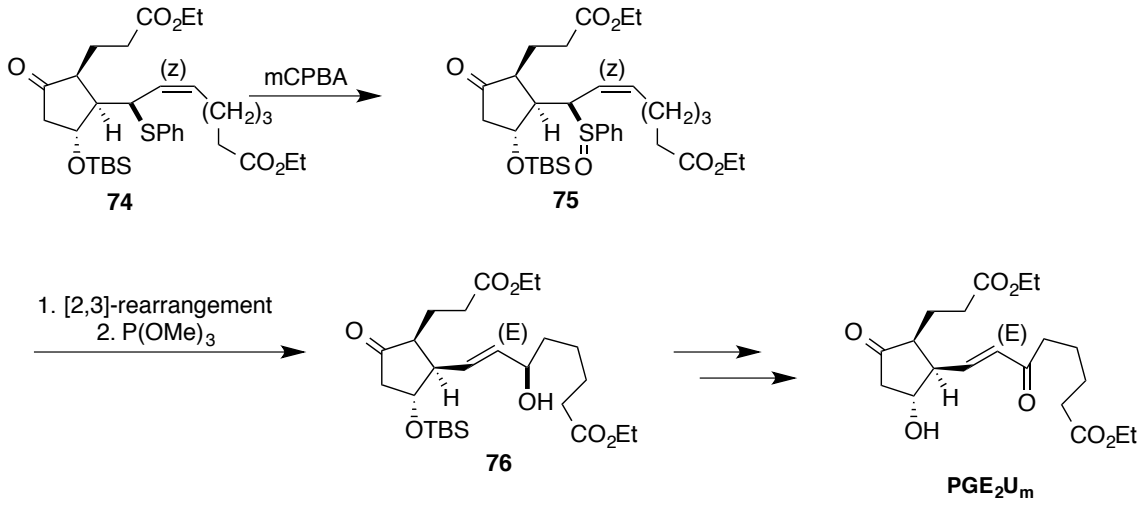


Figure 2-11. Tandem [2,3]-Wittig and oxy-cope rearrangement. Brevicomine and oxocrinal were synthesized by this tandem reaction sequence

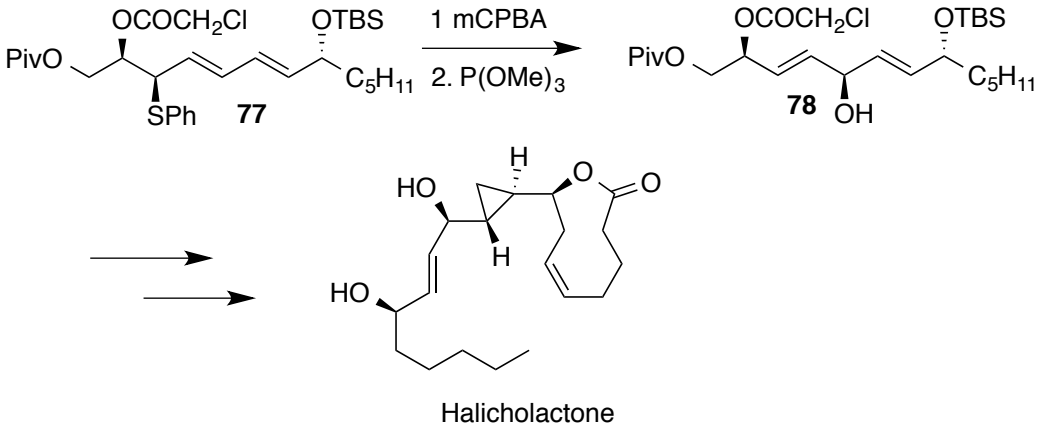
Besides Sommelet-Hauser and Wittig rearrangements synthetic chemists have used Mislow-Evans rearrangement extensively. There are many literature reports of total synthesis of natural products where Mislow-Evans rearrangement has been used in one of the key steps. One of the most important examples is the use of Mislow-Evans rearrangement during the total synthesis of the ethyl ester of the major urinary metabolite of Prostaglandin E_2 (PGE_2U_m) (Scheme 2-22).[106] The employment of Mislow-Evans rearrangement in this case particularly important as Mislow-Evans rearrangement showed very high E-selectivity, required for efficient synthesis of the natural product.

Scheme 2-22



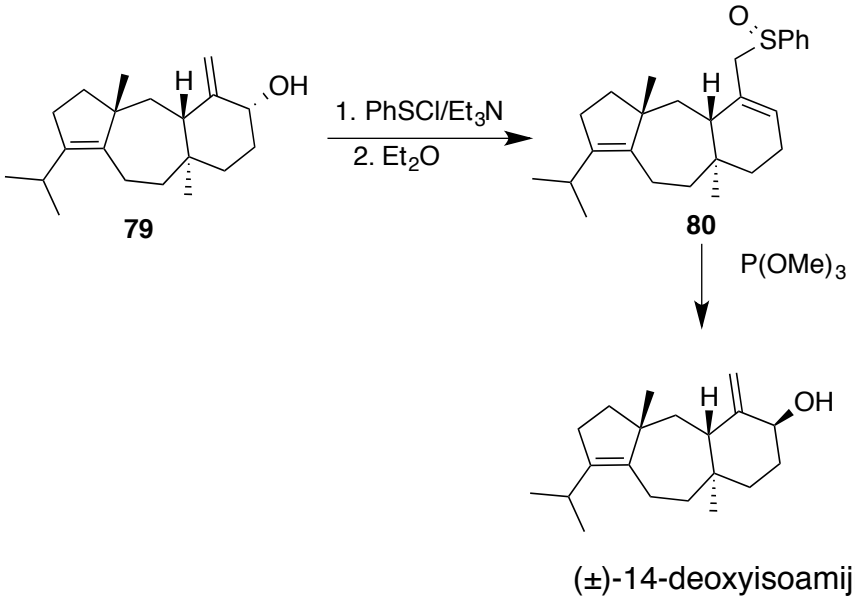
Tanaka exploited the high E-selectivity of Mislow-Evans rearrangement during the synthesis of Halicholactone (Scheme 2-23).[107]

Scheme 2-23



One of the most significant examples of synthetic utilities of Mislow-Evans rearrangement is its employment at the last step of total synthesis of (±)-14-deoxyisoamijiol.[108] Mitsunobu reaction gave poor yield at the last step of the synthesis. Then Mislow-Evans rearrangement was employed to achieve the desired molecule with considerably high yield (Scheme 2-24).

Scheme 2-24



79 **80** (±)-14-deoxyisoamijiol

The above discussions indeed exemplified the utility of [2,3]-rearrangement in synthetic organic chemistry.

Mechanistic Study on [2,3]-Sigmatropic Rearrangement

Due to its profound synthetic utilities, the mechanism of [2,3]-sigmatropic rearrangement has been studied extensively by many scientists.

According to Woodward-Hoffmann's pericyclic rule concerted [2,3]-sigmatropic rearrangement is an allowed pericyclic process.[27] This could be explained by the frontier molecular orbital (FMO) theory, developed by Fukui (Figure 2-12). The FMO interaction could be described as an interaction between LUMO of allyl anion and HOMO of the inium ($R_2C{=}N^+ R'_2$). Since all the interactions are "bonding" the [2,3]-rearrangement is an allowed pericyclic process.

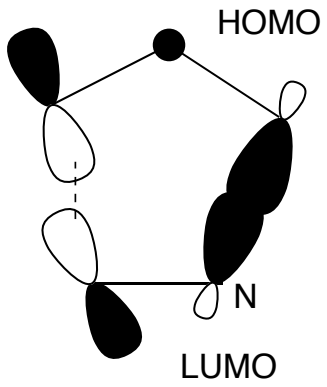


Figure 2-12. FMO analysis of concerted [2,3]-rearrangement

This concerted process rightly justifies the striking high yield and stereospecificity of [2,3]-sigmatropic rearrangement. Initially, the mechanistic study was

solely based on experiments. In 1972, Sharpless settled the debate regarding the mechanism of oxidation of alkenes by selenium dioxide. His mechanistic study suggested that organo-selenic acid-Se (IV) undergoes [2,3]-sigmatropic rearrangement to afford selenium ester-Se (II).[98] The possibility of alternative solvolysis pathway to form selenium ester Se (II) was rejected by confirming the absence of methyl ester in presence of methanol in the reaction medium. The concerted path for [2,3]-sigmatropic rearrangement has been supported by many experiments. For example, **cis-81** gives [2,3]-rearranged product while **trans-81** gives exclusively [1,2]-product (Figure 2-13). The inability of the trans isomer to undergo [2,3]-rearrangement strongly suggests that [2,3]-rearrangement is associated with a cyclic transition state.[35]

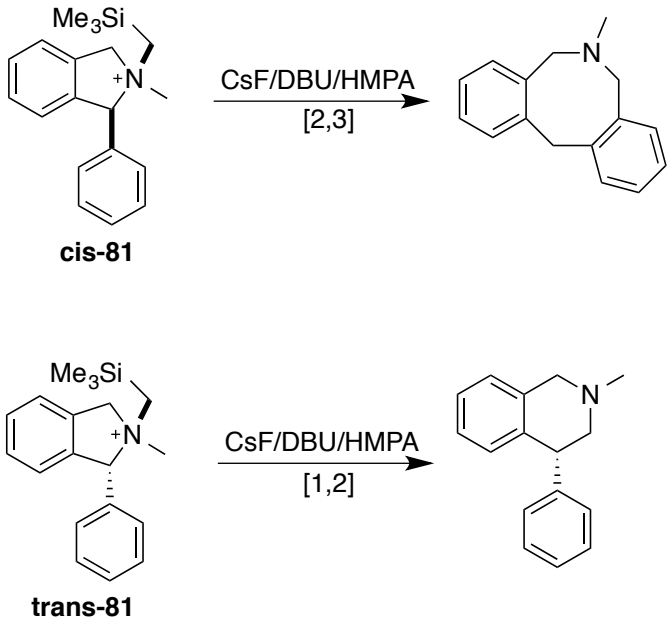


Figure 2-13. Selectivity of cis-81 and trans-81 towards sigmatropic rearrangement

With the advent of computational chemistry, researchers started to study [2,3]-rearrangement by theoretical calculations. Jursic studied [2,3]-rearrangement of ylides (nitrogen and sulfur) by *ab initio* method.[109] In his work, he judged two mechanistic possibilities for [2,3]-rearrangement. The first one is an ion pair mechanism the other is a concerted mechanism. The results of the theoretical calculations suggested that concerted mechanism is favored over the ion pair mechanism. The study also suggested that the rearrangement is associated with low energy barrier. This could be understood from the fact that the ylides are less stable compared to the rearranged products (either amines or sulfides). In 1991, Houk investigated [2,3]-rearrangement of sulfur ylides. Based on cyclic TSs for [2,3]-sigmatropic rearrangement his work successfully explained the stereochemical outcome of the rearrangement.[110] His study suggested that the stereochemical outcome of rearrangement of [2,3]-sigmatropic rearrangement results from ring strain, and the preference of the exo/endo-orientation of the lone pair on the sulfur atom associated with it. When there is an electron-withdrawing group adjacent to the carbon bearing the negative charge, the sulfur lone pair prefers to adopt endo disposition yielding Z-double bond. While in case of an electron releasing group, the lone pair prefers exo orientation resulting E-double bond. Figure 2-14 shows that when R=H, Me **trans-83** is the major product while R=CHO **cis-83** is preferred.

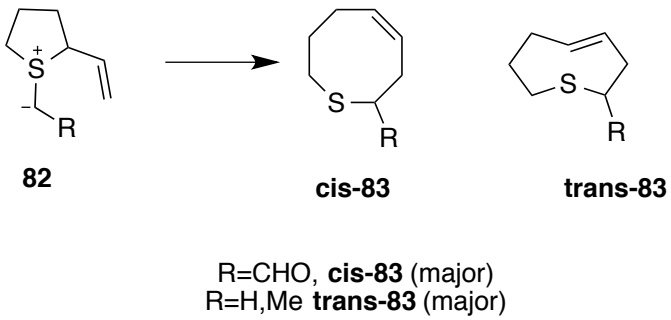


Figure 2-14. Stereoselectivity of [2,3]-rearrangement of 82

Jorgensen computationally studied Mislow-Evans rearrangement. His work was successfully able to rationalize the E-selectivity of Mislow-Evans rearrangement based on the relative energy of the competing transition states.[111]

Competition of [2,3]- and [1,2]-Rearrangement

However, the most interesting mechanistic question related to [2,3]-sigmatropic rearrangement is its competition with the [1,2]- sigmatropic rearrangement. In the realm of sigmatropic reactions, concerted [2,3]-sigmatropic rearrangement is an allowed pericyclic process while the concerted [1,2]-variety is a forbidden process. This could easily be understood by the FMO theory. The Figure 2-15 shows the FMO interaction for concerted [1,2]-rearrangement. Since the interaction for geometrically feasible concerted [1,2]-rearrangement is anti-bonding in nature the concerted [1,2]-rearrangement with retention is forbidden. The concerted [1,2]-rearrangment with inversion is allowed if only orbital interactions are considered. However, the concerted [1,2]-rearrangment with inversion is geometrically unfeasible.

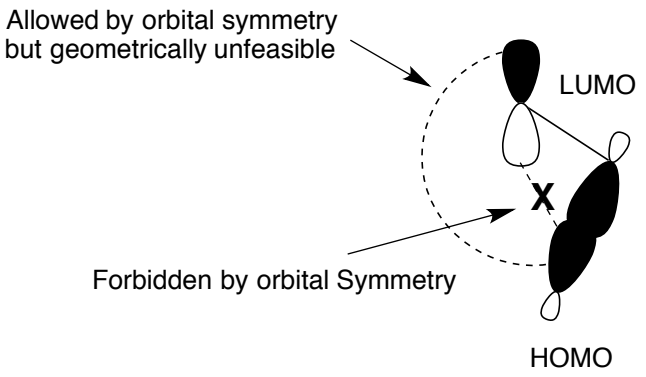


Figure 2-15. FMO analysis of concerted [1,2]-rearrangement

Interestingly, there are many literature reports about the co-occurrence of [2,3]- and [1,2]-rearrangement.[112] This is mechanistically intriguing as such competition between an allowed and forbidden pericyclic process is extremely rare. From a synthetic viewpoint, this competition limits the utility of [2,3]-rearrangement.

The traditional approach to explain this competition is that [2,3]-sigmatropic rearrangement is a concerted pericyclic process while [1,2]-variety is a stepwise process involving a cleavage-recombination mechanism. The concerted path is enthalpically favored, while the stepwise mechanism involving dissociation has an entropic advantage. Figure 2-16 depicts the traditional explanation for the competition. The blue line shows the concerted [2,3]-rearrangement path and the green line depicts the stepwise cleavage-recombination mechanism for formation of [1,2]-product. According to the traditional explanation the relative ratio of [2,3]- and [1,2]-product will be governed by the relative free energy of [2,3]-TS and [1,2]-TS (Figure 2-16).

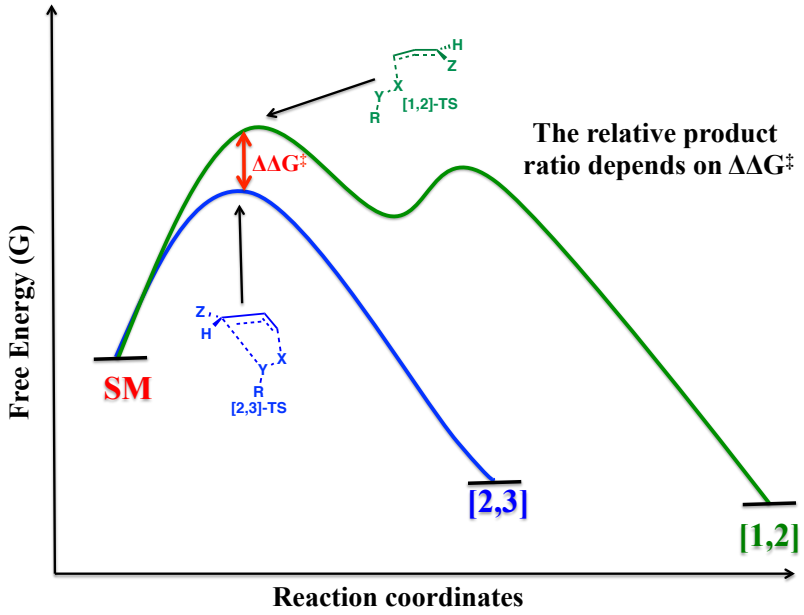


Figure 2-16. TST explanation of co-occurrence of [2,3]- and [1,2]-rearrangements

This explanation was supported by the fact that elevated temperatures favor entropically favored [1,2]-rearrangement over enthalpically favored [2,3]-rearrangement. Based on this traditional approach computational studies have been done to rationalize the experimentally observed product distribution. In 1996, Yates computationally investigated the competitive [2,3]- and [1,2]-rearrangement of N-methyl-3-propenylammonium methylide.[34] The study suggested that energy difference of the TSs associated with the rearrangements is very low (~0.5 kcal/mol). However, the system theoretically studied has never been studied experimentally. In 2010, Ghigo published a far more detailed study regarding the competition.[18] However, the study was not able to explain the experimentally observed [2,3]- and [1,2]-product distribution. Since the relative energy of the TSs could not account for the product distribution we envisioned

that the relative energy of the competing TSs might not be responsible for the pervasive competition.

Previously reported TSs for [2,3]-rearrangement suggested that the TS for this rearrangement is early and loose.[18, 34] We envisioned that dynamic effect might be responsible for this competition. Our hypothesis has been that this competition arises from the entropic bifurcation dynamic effect and not from the competing TSs. In detail, according to our hypothesis the competition of the concerted path and cleavage path does not result from the competing TSs. The competition results from partitioning of the dynamic trajectories from the pericyclic [2,3]-TS leading to concerted as well as cleavage path. In the following chapters we will discuss about the study that has been carried out to investigate the hypothesis.

CHAPTER III

EXPERIMENTAL AND THEORETICAL STUDY OF ^{13}C-KIES OF [2,3]-REARRANGEMENT OF AN ALLYL AMMONIUM YLIDE*

In the previous chapter we hypothesized that the competition between the allowed [2,3]- and forbidden [1,2]- process is due to the bifurcation of dynamic trajectories from the [2,3]-sigmatropic rearrangement TS. In order to mechanistically investigate our hypothesis we sought an in depth study of [2,3]-sigmatropic rearrangement. As we hypothesized that both the concerted and cleavage processes arise from the same [2,3]-TS we required very detailed structural information about this TS.

As it was already mentioned in CHAPTER I, KIEs give information about the geometry of the TS of a reaction, we envisioned that measuring KIEs of [2,3]-rearrangement process would be extremely helpful for our mechanistic study. In case of [2,3]-sigmatropic rearrangement four atoms are directly involved in σ-bond making and breaking process so we required KIEs at multiple positions. For this reason, Singleton's NMR methodology for measurement of KIEs at natural abundance was employed for measuring these KIEs. Also, it is possible to predict KIEs theoretically from computationally located TSs. We envisioned that both the experimental KIEs and theoretically predicted KIEs would be important for understanding the [2,3]-sigmatropic

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* Part of the data reported in this chapter is reprinted with permission from "Dynamics and a Unified Understanding of Competitive [2,3]- and [1,2]-Sigmatropic Rearrangements Based on a Study of Ammonium Ylides" by Biswas, B.; Collins, S. C.; Singleton, D. A. *J. Am. Chem. Soc.* **2014**, *136*, 3740-3743, Copyright [2014] by American Chemical Society.

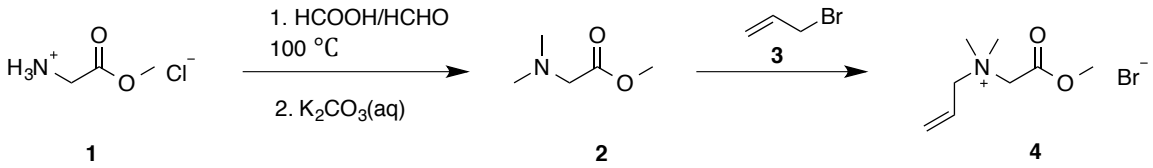
rearrangement. In this chapter a combined experimental and theoretical study of KIEs of [2,3]-sigmatropic rearrangement of an ammonium ylide will be discussed.

Experimental Results and Discussions

Coldham has reported the facile [2,3]-rearrangement of N-allyl α-aminoester ylides. In his work he used a comparatively weak base DBU (1,8-Diazabicyclo[5.4.0]undec-7-ene) to deprotonate the acidic hydrogen of the ammonium salt.[79] This is indeed very important for our purpose because use of a weak base will make the deprotonation step a reversible one and hence the subsequent rearrangement step will be the rate limiting step. This means that the experimental KIEs will correspond to the KIEs of the rearrangement step.

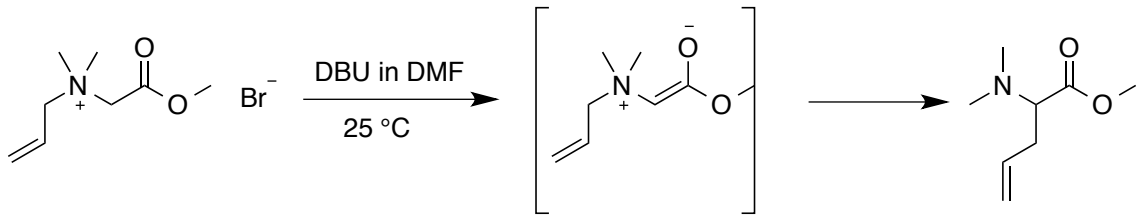
In Coldham's work, the ammonium salt was generated and subsequently rearranged in one pot. However for our purpose isolation of the ammonium salt was necessary because for measuring experimental KIEs, the initial isotopic compositions of the starting material for the sample and the standard have to be same. This requires same starting material for preparation of samples and standards. To accomplish this, N,N-dimethylglycine methyl ester **2** was synthesized from glycine methyl ester hydrochloride salt **1** employing the Eschweiler-Clarke reaction. Subsequent reaction of **2** with allyl bromide (**3)** affords desired ammonium salt (**4**).

Scheme 3-1



In the original study, the based mediated rearrangement (Scheme 3-2) was carried out at 40°C. However it has been found that the reaction goes smoothly at room temperature. For experimental simplicity the reaction was done at room temperature in DMF since KIEs are dependent on temperature and it is always easier to maintain room temperature as the reaction temperature than any other temperatures. Due to high hygroscopicity of the ammonium salt and its subsequent decomposition, probably due to hydrolysis of the methyl ester, the reaction required considerably dry condition. For this reason, the base mediated rearrangement was done in presence of 4 Å molecular sieves. Due to the possibility of starting material decomposition, trans-stilbene was included as an internal standard to quantify the conversion of the starting material to the product. Since it was impossible to recover the starting material, ammonium salt, KIEs were measured on the product, amine. There must be two reactions for each set of measurements; one reaction is for sample preparation where starting material ammonium salt (**4)** would be partially (15-20%) converted to **5** by using sub-stoichiometric amount of DBU. In another reaction **4** would be quantitatively converted to **5** using excess of DBU. This would serve as the "standard".

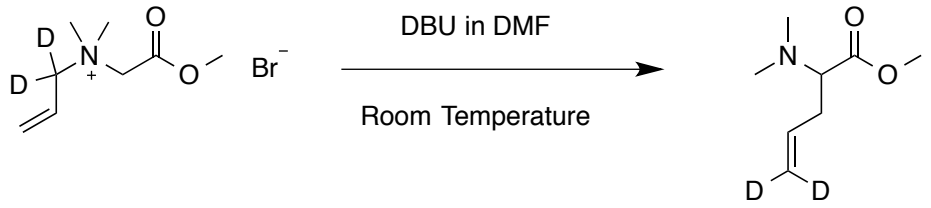
Scheme 3-2



4 **4'** **5**

Before measuring the experimental KIEs for [2,3]-rearrangement two important possibilities should be considered. First, for the system under study, [2,3]- and [1,2]-products are identical. So it might be possible that the product **5** might be obtained by [1,2]-process. If the competing [1,2]-path exists during the rearrangement we will no longer be able to treat the experimental KIEs obtained from product **5** as exclusive KIEs for [2,3]-sigmatropic rearrangement of **4′.** However, exclusive [2,3]-rearrangement of **4** under the reaction condition was confirmed by analyzing DBU-mediated rearrangement of **4-d$_2$** (Scheme 3-3).

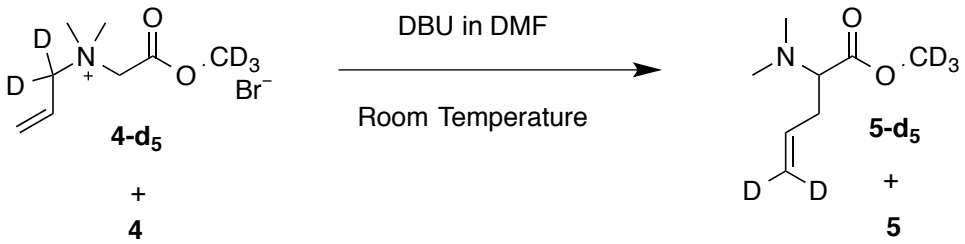
Scheme 3-3



4-d_2 **5-d_2 (only)**

Secondly, it might be possible that the [2,3]-rearrangement occurs partially via stepwise cleavage/recombination mechanism. In order to check the possibility of stepwise cleavage/recombination [2,3]-rearrangement a crossover experiment on an equimolar mixture of **4-d_5** and **4** was carried out (Scheme 3-4). The reaction mixture was analyzed by ESI-MS. No signals associated with crossover products [(M+2), (M+3)] have been detected. Absence of the crossover products ruled out the possibility of intermolecular [2,3]-rearrangement path.

Scheme 3-4



4-d_5

+

4

5-d_5

+

5

As there is no evidence of stepwise cleavage/recombination mechanism for rearrangement of **4′** we could rightly assume that the rearrangement of **4′** to **5** is exclusively a concerted [2,3]-rearrangement.

Experimental Kinetic Isotope Effects

As mentioned earlier, the recovery of the starting ammonium salt (**4**) is very difficult; we sought to measure the KIEs on product, **5**. Two sets of KIEs had been measured. For the first set the conversion for the sample was 11.7% while for the second sample the conversion was 21.3%. The ^{13}C abundance at each carbon in sample-**5** (obtained via low conversion of **4** to **5** using 15-20% of DBU) was compared with ^{13}C abundance in standard-**5** (obtained by 100% conversion of **4 to 5** using excess of DBU) by standard NMR methodology.[32] As the methoxy group of the ester is far from the reaction center it was assumed that isotopic composition of the methoxy carbon does not change during the course of the reaction. So the kinetic isotope effect was assumed to be 1.000 for methoxy carbon and the KIEs at the other positions have been measured with respect to that carbon using the equation (3-1). The experimental KIEs are shown in the Figure 3-1.

$$KIE_{SM(intermolecular)} = \log(1-F)/\log(1-F)*(R/R_0)] \qquad (3\text{-}1)$$

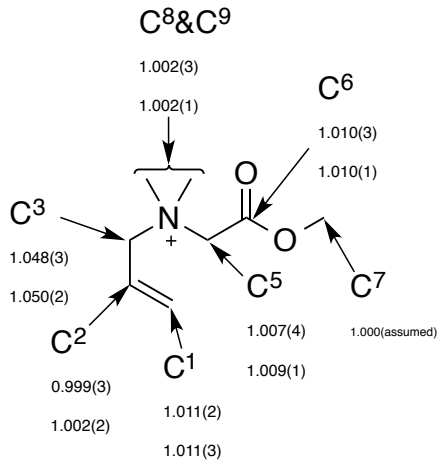


Figure 3-1. Experimental KIEs of [2,3]- rearrangement of **4**.

The result showed KIE on C^5 is not very large and considerable KIEs on other carbons. This indicates that the rearrangement step, and not the deprotonation step is the rate-limiting step. The experimental KIEs also indicate that the carbon (C^3) associated with the bond breaking process during the rearrangement has large (~5%) KIE while the carbons (C^1 and C^5) associated with bond making process have small KIEs (~1%).

The experimental KIEs suggest that at the transition state the bond breaking is more important than bond the formation. In other words the TS for the rearrangement is early and "loose".

Theoretical Calculations and Discussions

The experimental KIEs provided qualitative information about the TS geometry. However for in depth study of the reaction, we sought to probe the reaction with

theoretical calculations. With experimental KIEs in hand we decided to predict KIEs for rearrangement of **4′** to **5**. As the ammonium salt undergoes exclusive [2,3]-rearrangement the experimental KIEs could be predicted by locating the [2,3]-rearrangement TS. Firstly, KIEs were predicted by TST. The predicted KIEs based on TST differ considerably depending on the method employed. For example M062X located the tightest TS among all the methods employed while B97D located the loosest one.

In neither of the cases the predicted KIEs were not in good agreement with the experimental results. However, one key feature about the predicted KIEs is that, for all methods predicted KIEs at C^3 is large while at C^5 and C^1 the values were small. In other words all methods qualitatively predicted the experimental KIEs successfully. These values indeed indicate early and loose TS.

Even though most of the predicted KIEs were fairly in agreement with experimental KIEs the experimental KIEs suggested even an earlier TS compared to the TS predicted by TST. This suggests that the TSs located by TST are not adequate to predict the experimental results. In order to get more accurate results we decided to include corrections for canonical variational transition state theory (CVTST) effects and small curvature tunneling (SCT). Theoretical calculations indicated that the variational transition state (VTS) is appreciably earlier compared to the conventional TS indicating a significant effect of entropy. The theoretically predicted KIEs including the correction of CVT and SCT are listed in Table 3-1.

Table 3-1. KIEs predictions (25 °C, k_{12C}/k_{13C}) versus C^3-N and C^1-C^5 distances

Method	Basis Set	Solvent Model	C^3-N distance	C^1-C^5 distance	C^5 KIE	C^3 KIE	C^1 KIE	C^6 KIE
wB97	6-31G*	PCM	1.90	2.28	1.023	1.042	1.021	1.008
M11	6-31G*	PCM	1.96	2.36	1.017	1.040	1.019	1.009
wB97X	6-31G*	PCM	1.99	2.40	1.018	1.044	1.018	1.008
lc-B97D	6-31G*	PCM	2.07	2.42	1.019	1.043	1.020	1.010
wB97X	6-31+G**	PCM	2.04	2.43	1.017	1.045	1.018	1.011
M11	6-31G*	gas phase	1.948	2.435	1.015	1.040	1.017	1.007
M06-2X	6-31+G**	PCM	2.03	2.46	1.015	1.045	1.017	1.011
SOGGA11X	6-31G*	PCM	2.04	2.51	1.016	1.046	1.017	1.009
wB97XD	6-31G*	PCM	2.04	2.51	1.015	1.045	1.017	1.009
wB97XD	6-31+G**	PCM	2.09	2.53	1.015	1.045	1.018	1.011
M06-2X	6-31+G**	GAS	1.999	2.534	1.014	1.045	1.016	1.008
N12SX	6-31G*	PCM	2.032	2.55	1.013	1.047	1.016	1.009
PBE0-D3	6-31G*	PCM	2.028	2.57	1.013	1.046	1.016	1.009
SOGGA11X	6-31G*	gas phase	2.014	2.578	1.014	1.047	1.015	1.007
PBE0	6-31+G**	PCM	2.073	2.593	1.012	1.049	1.015	1.011
WB97XD	6-31+G**	gas phase	2.048	2.6	1.012	1.048	1.014	1.008
M06-D3	6-31G*	PCM	2.098	2.609	1.012	1.047	1.015	1.010
N12SX	6-31G*	gas phase	1.997	2.617	1.012	1.047	1.014	1.007
MN12SX	6-31G*	PCM	2.111	2.623	1.012	1.049	1.016	1.010
APFD	6-31G*	PCM	2.045	2.625	1.015	1.044	1.016	1.007
PBE0-D3	6-31G*	gas phase	1.991	2.642	1.012	1.047	1.014	1.007
M06	6-31+G**	PCM	2.14	2.65	1.010	1.050	1.014	1.011
M06-D3	6-31G*	gas phase	2.064	2.66	1.011	1.047	1.014	1.007
PBE0	6-31+G**	GAS	2.029	2.665	1.01	1.049	1.014	1.008
APFD	6-31G*	gas phase	2.001	2.684	1.011	1.053	1.010	1.005
MN12SX	6-31G*	gas phase	2.076	2.684	1.012	1.049	1.014	1.008

Table 3-1. Continued

Method	Basis Set	Solvent Model	C^3-N distance	C^1-C^5 distance	C^5 KIE	C^3 KIE	C^1 KIE	C^6 KIE
B98	6-31G*	PCM	2.09	2.70	1.011	1.046	1.015	1.010
B3LYP-D2	6-31G*	PCM	2.115	2.708	1.011	1.046	1.015	1.009
M06	6-31+G**	GAS	2.084	2.708	1.009	1.051	1.012	1.008
B972	6-31G*	PCM	2.08	2.71	1.011	1.048	1.014	1.010
B3LYP-D2	6-31+G**	SMD	2.14	2.72	1.012	1.049	1.015	1.012
MN12L	6-31G*	PCM	2.182	2.723	1.012	1.051	1.015	1.010
B3LYP-D2	6-31+G**	PCM	2.15	2.73	1.010	1.047	1.015	1.011
B971	6-31+G**	PCM	2.128	2.729	1.011	1.047	1.016	1.011
B98	6-31+G**	PCM	2.13	2.73	1.011	1.046	1.016	1.012
B972	6-31+G**	PCM	2.112	2.74	1.009	1.050	1.014	1.012
M11L	6-31G*	PCM	2.127	2.756	1.010	1.052	1.017	1.011
BP86-D2	6-31G*	PCM	2.077	2.769	1.010	1.045	1.014	1.008
B3LYP-D3	6-31G*	PCM	2.102	2.77	1.011	1.046	1.014	1.010
PBEPBE-D2	6-31G*	PCM	2.06	2.776	1.009	1.046	1.013	1.008
MN12L	6-31G*	gas phase	2.125	2.777	1.011	1.051	1.013	1.008
B3LYP-D2	6-31G*	gas phase	2.062	2.789	1.010	1.047	1.013	1.007
B3LYP	6-31G*	PCM	2.103	2.791	1.010	1.048	1.013	1.010
B971	6-31+G**	gas phase	2.067	2.816	1.009	1.049	1.012	1.008
B3LYP	6-31+G**	PCM	2.14	2.82	1.009	1.049	1.013	1.012
B972	6-31+G**	gas phase	2.045	2.822	1.009	1.050	1.012	1.009
M11L	6-31G*	gas phase	2.092	2.823	1.009	1.052	1.016	1.009
N12	6-31+G**	PCM	2.07	2.836	1.007	1.051	1.011	1.011
B3LYP-D3	6-31G*	gas phase	2.038	2.864	1.010	1.046	1.012	1.007
N12	6-31G*	gas phase	1.977	2.869	1.008	1.050	1.0091	1.007
BP86-D2	6-31G*	gas phase	1.985	2.88	1.008	1.046	1.010	1.006
PBEPBE-D2	6-31G*	gas phase	1.978	2.88	1.008	1.047	1.010	1.006

Table 3-1. Continued

Method	Basis Set	Solvent Model	C^3-N distance	C^1-C^5 distance	C^5 KIE	C^3 KIE	C^1 KIE	C^6 KIE
B97D	6-31G*	PCM	2.04	2.96	1.008	1.048	1.0087	1.009
B97D	6-31+G**	PCM	2.063	2.965	1.007	1.049	1.009	1.010
SOGGA11	6-31G*	PCM	2.04	2.97	1.007	1.045	1.013	1.009
B97D	6-31+G**	PCM	2.06	2.97	1.007	1.049	1.0089	1.011
B97D3	6-31G*	PCM	1.953	3.001	1.008	1.050	1.005	1.009
B97D	6-31+G**	gas phase	1.911	3.056	1.007	1.049	1.006	1.007
BLYP-D2	6-31G*	gas phase	1.862	3.062	1.008	1.046	1.005	1.006
SOGGA11	6-31G*	gas phase	1.951	3.135	1.007	1.046	1.008	1.007
B971	6-31G*	PCM	2.08	2.70	1.011	1.046	1.015	1.010
B3LYP	6-31+G**	gas phase	2.058	2.911	1.008	1.049	1.011	1.009
BLYP-D2	6-31G*	PCM	2.061	2.953	1.008	1.047	1.009	1.008

Conclusion

The experimental KIEs provided information about the TS structure of the base mediated [2,3]- rearrangement of **4**. The experimental results suggested that the TS is early and loose. The reaction was further investigated by theoretical calculations. The predicted KIEs based on TST were in fairly good agreement with experimental values. Irrespective of the method used, the located TS was early and loose. Among those methods B3LYPD2/6-31+G**/PCM was the best one to predict experimental KIEs. However, a better agreement with experimental values has been achieved by predicting KIEs using CVTST. The necessity of employing of CVTST for better prediction

suggested that the effect of entropy is significant. The effect of entropy was further supported by the fact that the TS located by CVTST is appreciably earlier than the TS located by TST. The agreement between experimental KIEs with theoretically predicted KIEs successfully probe the [2,3]-rearrangement of base induced ammonium salt **4**.

Our final goal is to unravel the origin of competition between formally allowed [2,3]- and formally forbidden [1,2]-rearrangement. However, the system we studied does give solely [2,3]-product. Even though the system under study did not give any [1,2]-product the study provided the information about the [2,3]-rearrangement TS geometry. In addition, the necessity of using CVTST for more accurate theoretical prediction of KIEs also suggests that effect of entropy is significant. The TS located by CVTST is earlier than the TS located by TST. This suggests that the TS is somewhat dissociative in nature. In conclusion, the study discussed in the chapter is indeed an important step to unravel the origin of the competition between an "allowed" [2,3]-rearrangement and "forbidden" [1,2]-rearrangement.

Experimental Procedures

General Comment

All glassware, magnetic stirring bars, and molecular sieves used in these reactions were oven-dried overnight.

Acknowledgement

I am really grateful to my former group member Sean C. Collins who measured the experimental KIEs of DBU-mediated sigmatropic rearrangement of **4**.

*Synthesis of **4***

To a 250-mL round-bottomed flask containing 19.07 g (163 mmol) of 4 were added 40 mL of acetonitrile, and then the sample was dissolved to form a solution. Then 19.72 g (163 mmol) of allyl bromide were added and the reaction mixture stirred with a magnetic stirrer at room temperature (r.t.) for 20 h. The solution was concentrated under reduced pressure until **4** was crystallized as an off-white solid. ^{1}H-NMR analysis was carried out to characterize **4** and compared with reported ^{1}H-NMR of **4**.[79] The isolated yield of **4** was found to be 27.15 g (114 mmol, 70%)

General Procedures for DBU-induced Rearrangements

All glassware, magnetic stirring bars, and molecular sieves used in these reactions were oven-dried overnight. Solvent was dried using 4 Å molecular sieves.

*DBU-induced Rearrangement of **4** – Sample*

Trans-stilbene (1.81 g, 10.0 mmol, internal standard) and **4** (20.18 g, 84.8 mmol) were dissolved in 25 mL of DMF, then DBU (1.98 g, 14.8 mmol) and 24 g of 4 Å powdered molecular sieves were added and the mixture was left stirring for 30 min at 25 °C, allowing the reaction to proceed to 11.7% conversion. The reaction mixture was

diluted with 40 mL of $CHCl_3$ and 70 mL of water, and then the aqueous layer was extracted twice with 70 mL of $CHCl_3$. The organics were washed with 50 mL of water, dried with Na_2SO_4, and concentrated under reduced pressure. The residual organics were dissolved in 150 mL of Et_2O, washed twice with 50 mL of water, then dried with Na_2SO_4 and concentrated under reduced pressure. The resulting crude mixture was purified by flash chromatography using 1% MeOH in DCM to afford 0.50 g (3.40 mmol, 4%) of **5**. ^{1}H NMR ($CDCl_3$): δ 2.26 (s, 6 H), 2.35 (m, 2 H), 3.1 (dd, 1 H), 3.6 (s, 3 H), 5.0 (m, 2 H), 5.7 (m, 1 H). ^{13}C NMR ($CDCl_3$): δ 33.7, 41.3, 50.6, 67.2, 116.8, 134.0, 171.7.

*DBU-induced Rearrangement of **4** – Standard*

Trans-stilbene (0.92 g, 5.1 mmol, internal standard) and **4** (3.57 g, 15 mmol) were dissolved in 15 mL of DMF, then 9.13 g (60 mmol, 4 eq.) of DBU and 12 g of 4 Å powdered molecular sieves were added and the mixture left stirring for 3h at r.t., allowing the reaction to proceed to 100% conversion. The reaction mixture was diluted with 50 mL of $CHCl_3$ and 70 mL of water, and then the aqueous layer was extracted twice with 70 mL of $CHCl_3$. The organics were washed with 50 mL of water, dried with Na_2SO_4, and concentrated under reduced pressure. The residual organics were dissolved in 150 mL of Et_2O, washed twice with 50 mL of water, then dried with Na_2SO_4 and concentrated under reduced pressure. The resulting crude mixture was purified by flash chromatography using 1% MeOH in DCM to afford 0.64 g (27%) of **5**.

In each case closely analogous reactions were carried out for duplicate

measurements of the KIEs. In the duplicate samples the conversion of the sample was 21.3%.

A note on spectra: we certify that all spectra presented are unaltered screen dumps or pdf printouts of the original spectra. Please note that scales are typically increased by a factor of 5 from normal to show impurities clearly. The raw electronic files are saved and always available on request from Dr. Daniel A. Singleton.

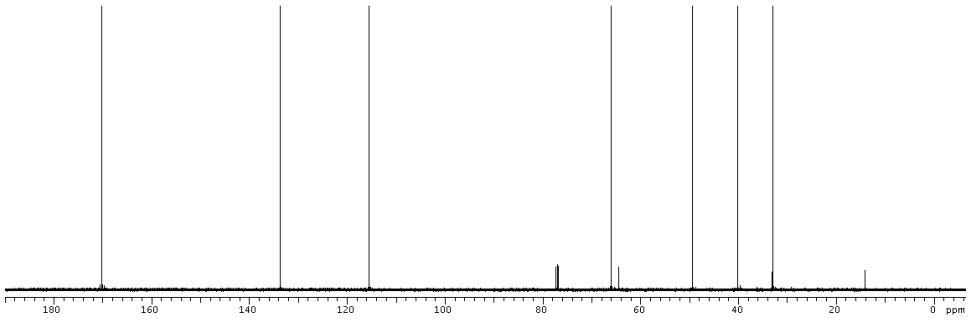


Figure 3-2. Sample ^{13}C NMR spectrum of sample. Partial conversion of **4** to **5**

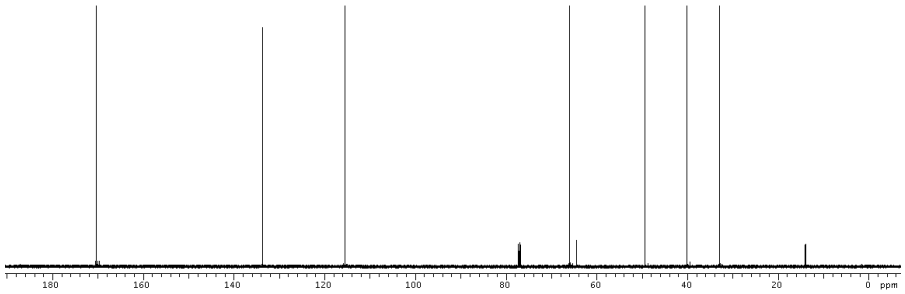


Figure 3-3. Sample ^{13}C NMR spectrum of standard. Quantitative conversion of **4** to **5**

NMR Measurements

All NMR samples consisted of approximately 400 mg of **5** in 5 mm NMR tubes filled to a constant height of 5 cm with $CDCl_3$. The ^{13}C spectra were recorded at 125.7 MHz using inverse gated decoupling, 75.5 s delays between calibrated $\pi/2$ pulses, and a 12 s acquisition time to collect 600,000 points. The integrations were obtained numerically by a procedure given in a macro provided in a later section. A zero-order baseline correction was generally applied, but to avoid any qualitative manipulation no first-order or higher-order baseline correction was ever applied. Six spectra were recorded for each sample and standard.

NMR Results and Calculation of KIEs

The raw integrations are shown in Table 3-2, along with average values and standard deviations. The integration of peak 5, the methyl-ester carbon, was in each case set to 1000.

Table 3-2. ^{13}C integrations for measurement of KIEs of rearrangement of **4′**.

SAMPLE2	Macro: macrokie2samp	File: SEAN-KIE2-SAMPLE-ERIK-CUT-OME						
Carbon	Spectra1	Spectra2	Spectra3	Spectra3	Spectra4	Spectra5	Avg.	SDev
C^1	1054.8	1052.3	1055.2	1053.6	1053.4	1054.6	1054.0	1.1
C^2	1020.7	1021.2	1022.5	1021.3	1020.8	1021.6	1021.4	0.7
C^3	950.5	950.9	952.6	949.1	950.7	949.6	950.6	1.2
C^5	992.0	991.6	991.1	992.7	991.8	992.3	991.9	0.6
C^7	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	0.0
C^8&C^9	1942.9	1942.8	1943.6	1941.3	1943.7	1943.8	1943.0	1.0
Standard2	Macro: macrokie2	File: SEAN-KIE2-STANDARD-ERIK-CUT-OME						
Carbon	Spectra1	Spectra2	Spectra3	Spectra3	Spectra4	Spectra5	Avg.	SDev
C^1	1063.2	1062.8	1063.1	1063.6	1064.4	1065.0	1063.7	0.9
C^2	1022.9	1021.5	1022.5	1022.9	1024.2	1026.2	1023.4	1.6
C^3	989.2	992.7	992.1	995.0	992.9	995.0	992.8	2.1
C^5	998.7	1000.0	998.0	999.4	1000.5	1000.5	999.5	1.0
C^6	996.9	999.2	996.7	1000.3	998.5	1000.6	998.7	1.6
C^7	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	0.0
C^8&C^9	1943.1	1945.9	1945.1	1946.9	1948.4	1948.9	1946.4	2.2
Sample1	macro: seankiesamp	File: SEAN-KIE-SAMPLE-ERIK-CUT						
Carbon	Spectra1	Spectra2	Spectra3	Spectra3	Spectra4	Spectra5	Avg.	StDev
C^1	1020.9	1022.4	1024.0	1025.4	1022.5	1026.4	1023.6	2.0
C^2	1022.7	1020.9	1021.3	1021.3	1022.2	1022.3	1021.8	0.7
C^3	947.7	944.9	949.0	947.4	951.8	948.1	948.2	2.2
C^5	985.5	983.3	980.4	986.6	984.9	986.5	984.5	2.4
C^6	978.1	978.6	973.6	978.7	977.3	980.9	977.9	2.4
C^7	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	0.0
C^8&C^9	1927.1	1922.0	1920.3	1926.8	1928.5	1933.6	1926.4	4.8

Table 3-2. Continued

Standard1	macro: seankiestd	File: SEAN-KIE-STANDARD-ERIK-CUT						
Carbon	Spectra1	Spectra2	Spectra3	Spectra3	Spectra4	Spectra5	Avg.	StDev
C^1	1033.5	1029.5	1033.8	1032.3	1033.0	1035.1	1032.9	1.9
C^2	1021.6	1018.5	1019.3	1018.4	1022.5	1025.2	1020.9	2.7
C^3	991.5	988.7	990.2	991.5	992.2	991.3	990.9	1.3
C^5	992.8	987.9	987.1	992.9	990.1	996.9	991.3	3.6
C^6	978.1	978.6	973.6	978.7	977.3	980.9	977.9	2.4
C^7	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	0.0
C^8&C^9	1927.1	1922.0	1920.3	1926.8	1928.5	1933.6	1926.4	4.8

The isotope effects were then calculated as:

KIE = ln(1-F)/ln(1-(F*IntSample/IntStandard))

Where F is the fractional conversion (0.117 for reaction 1, 0.213 for reaction 2), IntSample is the average integration for the sample for the carbon peak of interest in the table above, and IntStandard is the average integration for standard for the carbon peak of interest in the table above. For example, the KIE for carbon 1 of sample 2 /standard 2 was calculated as ln(1-0.213)/ln(1-0.213*1054.0/1063.7).

The uncertainties arising from uncertainties in F were negligible, and the major source of uncertainty is random variation in the integrations due to noise. For six measurements, the 95% confidence ranges in the average raw integrations are approximately the standard deviations shown in the table above, and the 95% confidence ranges for the KIEs were approximated as the square-root of the sum of the squares of the fraction uncertainties in the integrations. For example, the uncertainty for carbon 1

of sample 2 /standard 2 was calculated as $[(1.1/1054)^2 + (0.9/1063.7)^2]^{1/2}$

Synthesis of 2-Propen-1,1-d_2-1-ol and Allyl Bromide-d_2

To a mixture of 250 mL of diethyl ether (dried over sodium followed by distillation under nitrogen) and 2.50 g (60 mmol) of $LiAlD_4$ at 0 °C under nitrogen was added dropwise 9.05 g (100 mmol) of acryloyl chloride in 110 mL of dry ether. The mixture was allowed to stir overnight at room temperature then quenched by the successive addition of 2.5 mL of 15% aqueous sodium hydroxide, 7.5 mL of water and 2.5 mL of 15% aqueous sodium hydroxide at 0 °C. The reaction mixture was filtered and the filtrate was dried over anhydrous magnesium sulfate, and the volatiles were removed on a rotatory evaporator using an ice-water bath to afford 1.8 g (30 mmol, 30%) of crude propen-1,1-d_2-1-ol.

The crude material was used in the next step without further purification. The deuterated alcohol was used to synthesize d_2-allyl bromide using a reported procedure. The resulting ratio of **A** to **B** was found to be 9:1 by NMR analysis (Figure 3-4).

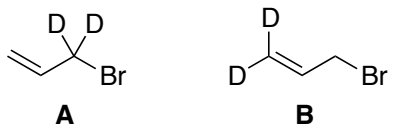


Figure 3-4. Structures of **A** and **B**

Synthesis of Methyl-d_3 Bromoacetate

To a mixture of 3.20 g (88.0 mmol) of d_4-methanol, 4.50 g (44.0 mmol) of triethylamine and 10 mL of dichloromethane (dried over 3Å molecular sieves) under nitrogen at 0° C was added dropwise slowly 8.80 g (43.96 mmol) of bromoacetyl bromide. The mixture was allowed to stir for 2 h, then quenched by the addition of 50 mL of 15% aqueous sulfuric acid at 0 °C. The organic layer was washed with two 25-mL portions of water and two 25-mL portions of saturated aqueous sodium bicarbonate solution. After drying over anhydrous magnesium sulfate the volatiles were removed on a rotatory evaporator to afford 6.1 g (39.56 mmol, 90%) of crude methyl-d_3 bromoacetate. ^{1}H NMR ($CDCl_3$): δ 3.84 (s).

Synthesis of N,N-dimethylglycine Methyl-d_3 Ester

A mixture of 10.00 g (88.89 mmol) of 40% aqueous solution of dimethylamine and 4 mL of acetonitrile was cooled to 0 °C in an ice-bath. After cooling the mixture, 6.00 g (38.5 mmol) of methyl-d_3 bromoacetate was added and the mixture was stirred at 0 °C for 12 h. The reaction mixture was then poured into 20 mL of water and the organics were extracted with three 50-mL portions of diethyl ether. The ether extracts were combined and dried over anhydrous sodium sulfate. The volatiles were then removed on a rotatory evaporator to afford 3.77 g (32.3 mmol, 84%) of *N*, *N*-dimethylglycine methyl-d_3 ester. ^{1}H NMR (399.53 MHz, $CDCl_3$): δ 2.33 (s, 6 H), 3.16 (s, 2 H),

*Ammonium Salt **4-d$_5$***

To a mixture of 292 mg (2.43 mmol) of N,N-dimethylglycine methyl-d_3 ester and 2 mL of ether (dried over sodium followed by distillation under nitrogen) under nitrogen at room temperature was added 300 mg (2.43 mmol) of d_2-allyl bromide. The resulting mixture was stirred overnight. During the stirring solid precipitated out from the solution. The volatiles were removed under vacuum to afford 459 mg (1.90 mmol, 78%) of crude ammonium salt **4-d$_5$** (**C** and **D**), judged to be more than 95% pure by comparing NMR of the unlabeled **4** (Figure 3-5). The ratio of **C** to **D** was found to be (10:7) by NMR analysis.

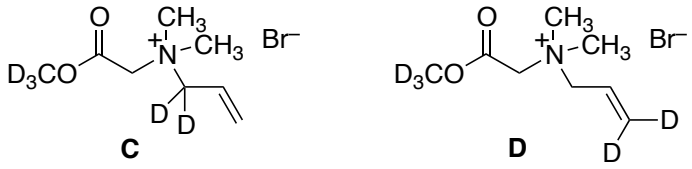


Figure 3-5. Structures of **C** and **D**

*Crossover Rearrangement of **4 / 4-d$_5$***

To a mixture of 249 mg (1.05 mmol) of **4**, 252 mg (1.05 mmol) of **4**-d_5 and 3.0 mL of N,N-dimethylformamide (dried over 3Å molecular sieves) under nitrogen at room temperature was added 600 mg (3.94 mmol) of DBU dropwise. The stirring of the reaction mixture continued for additional 1 h at room temperature before the reaction mixture was partitioned between 25 mL of ether and 25 mL of water. The ether layer

was washed with three 25-mL portions of water. Then the ether layer was dried over sodium sulfate. After removing the volatiles on a rotatory evaporator residue was analyzed by ^{1}H-NMR and ESI-MS. The M+3 peak that would be associated with crossover was not detectable in the ESI-MS.

Ammonium Salt ***4-d$_2$***

To a mixture of 680 mg (5.81 mmol) of N,N-dimethylglycine methyl ester and 5 mL of ether (dried over sodium followed by distillation under nitrogen) under nitrogen at room temperature was added 685 mg (5.57 mmol) of d_2 -allyl bromide. The resulting mixture was stirred overnight. During the stirring solid precipitated out from the solution. The volatiles were removed under vacuum to afford 748 mg (3.06 mmol, 55%) of crude ammonium salt **4**-d_2 (**E** and **F**), judged to be more than 95% pure by comparing NMR of the unlabeled **4** (Figure 3-6). The ratio of **E** to **F** was found to be (10:1) by NMR analysis.

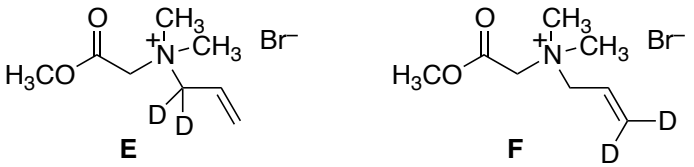


Figure 3-6. Structures of **E** and **F**

DBU Mediated Rearrangement of ***4-d₂***

To a mixture of 1.0 mL of N,N-dimethylformamide (dried over 3Å molecular sieves) and 238 mg (1.00 mmol) of **4**-d_2 (ratio of **E** to **F** is 10:1) under nitrogen at room temperature, was added 1.52 g (10.0 mmol) of DBU. The stirring of the reaction mixture continued for additional 1 h at room temperature before the reaction mixture was partitioned between 25 mL of ether and 25 mL of water. The ether layer was washed with three 25-mL portions of water. Then the ether layer was dried over sodium sulfate. After removing the volatiles on a rotatory evaporator the ratio of **G** to **H** was judged to be 10:1 from ^{1}H-NMR analysis (Figure 3-7).

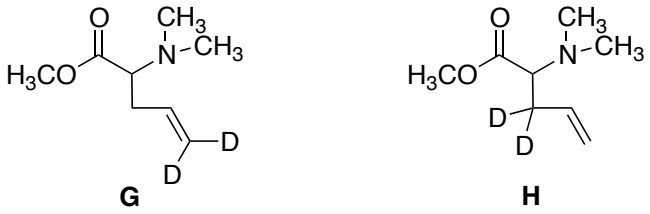


Figure 3-7. Structures of **G** and **H**

CHAPTER IV

STUDY OF COMPETITION BETWEEN [2,3]- AND [1,2]-REARRANGEMENT OF ALLYL YLIDES*

In the previous chapter we studied KIEs for the [2,3]-rearrangement of an ammonium ylide by a combination of experimental KIEs and theoretical calculations. The study revealed structural features of the TS for the [2,3]-sigmatropic rearrangement. The experimental results suggested that the reaction was associated with early an TS. This observation can be explained by Hammond's postulate. As the starting material (ylide) is of higher energy compared to the product (amine), the associated TS will be energetically and structurally similar to the starting material. Moreover, the KIEs at the carbon centers that are going to form the bond during the rearrangement process showed only 1% KIE. This suggests that the interaction between those carbon atoms is very weak at the TS. In addition, the KIEs predicted by the VTST are appreciably more accurate than those predicted by the TST. This indicated that the effect of entropy was significant during the rearrangement. Successful prediction of experimental results confirmed the reliability of theoretical calculations to model the [2,3]-sigmatropic rearrangements of ammonium ylides.

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* Part of the data reported in this chapter is reprinted with permission from "Dynamics and a Unified Understanding of Competitive [2,3]- and [1,2]-Sigmatropic Rearrangements Based on a Study of Ammonium Ylides" by Biswas, B.; Collins, S. C.; Singleton, D. A. *J. Am. Chem. Soc.* **2014**, *136*, 3740-3743, Copyright [2014] by American Chemical Society.

Even though our study successfully probed the [2,3]-rearrangement by a combination of experiments and theoretical calculations, our final goal was to rationalize the competition between the formally allowed [2,3]- and forbidden [1,2]-process. But, the system we studied gave the [2,3]-product exclusively. In order to achieve our final goal, we needed to find a system (ylide) that would give a mixture of products. We hypothesized that the competition between the formally allowed [2,3]-sigmatropic rearrangement and forbidden [1,2]-rearrangment results from the dynamic partitioning of trajectories from the [2,3]-rearrangement TS. In order to support our hypothesis, we ran dynamic trajectories on the [2,3]-sigmatropic rearrangement TS to predict the experimentally observed extent of cleavage. Also, we needed to test the traditional two-transition state hypothesis. According to that hypothesis, the relative amount of the [2,3]- and the [1,2]-product depends on the free energy difference between the [2,3]-TS and the cleavage-TS (Figure 4-1). We theoretically located those TSs and from their relative free energy we tested the hypothesis.

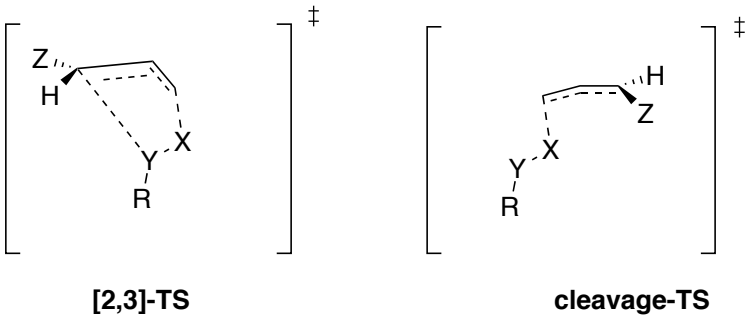
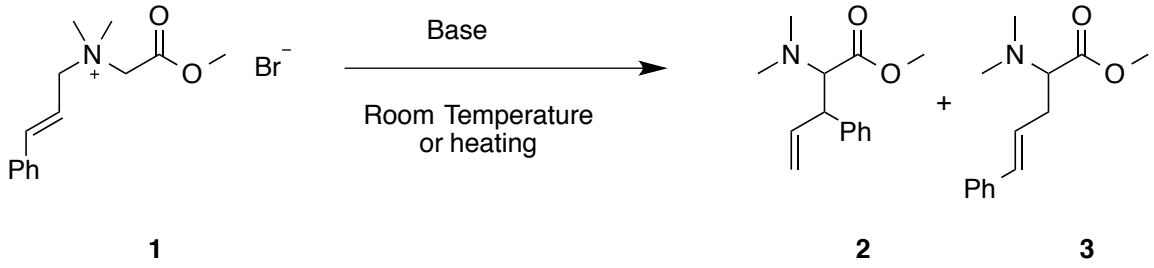


Figure 4-1. TSs of the [2,3]- and the [1,2]-sigmatropic rearrangement

Experimental Results and Discussions

In order to understand the origin of competition we sought to investigate systems similar to ammonium salt (**4**) in Chapter-III. Structurally similar ammonium salt **1** was first chosen for the study.[113]

Scheme 4-1



1 **2** **3**

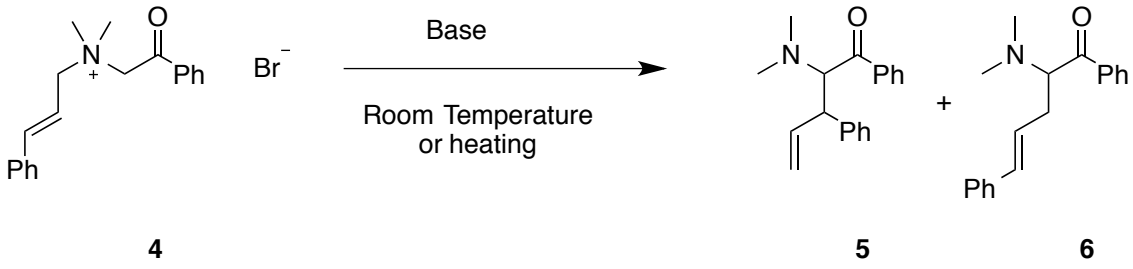
The ammonium salt (**1**) was first reacted with DBU in acetonitrile at room temperature. However, at room temperature, the salt exclusively formed the [2,3]-product **2**. As it is well known that higher temperatures favor the [1,2]-product, the ammonium salt was then treated with DBU at higher temperatures. Unfortunately in all cases, **1** afforded exclusively the product **2** ([2,3]-product). It is worthwhile to note that the reaction was not carried out at temperatures beyond 165 °C because around 200 °C the [2,3]-sigmatropic product (**2**) rearranges to the thermodynamically more stable [1,2]-product (**3**).[114]

As our first system (Scheme 4-1) failed to exhibit the desired competition, we

sought to screen several ammonium salts that could potentially exhibit the desired competition.

Stevens and his coworkers reported that **4** gave both the [2,3]- and [1,2]-rearranged products **5** and **6** respectively when treated with hydroxide base at an elevated temperature (Scheme 4-2).[115] Encouraged by their report we decided to study the DBU-induced rearrangement of **4.** But to our surprise, when treated with DBU, **4** only gave product **5** ([2,3]-product]) at room temperature. We further investigated the base-mediated rearrangement with KOH at elevated temperatures (60 °C and 80 °C). However, under all reaction conditions **4** failed to afford a mixture of the [2,3]- and [1,2]- products.

Scheme 4-2

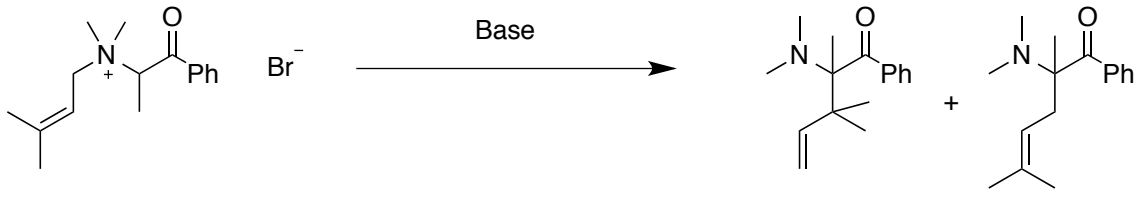


4 **5** **6**

Our result was supported by similar findings, from Ollis' group. They also failed to obtain any [1,2]-product from **4** when they treated **4** with methoxide as the base.[36]

However, Ollis and his coworkers reported that ammonium salt **7** on treatment with 10(N) aqueous sodium hydroxide gave both **8** ([2,3]-product) and **9** ([1,2]-product) at room temperature (Scheme 4-3).[36]

Scheme 4-3



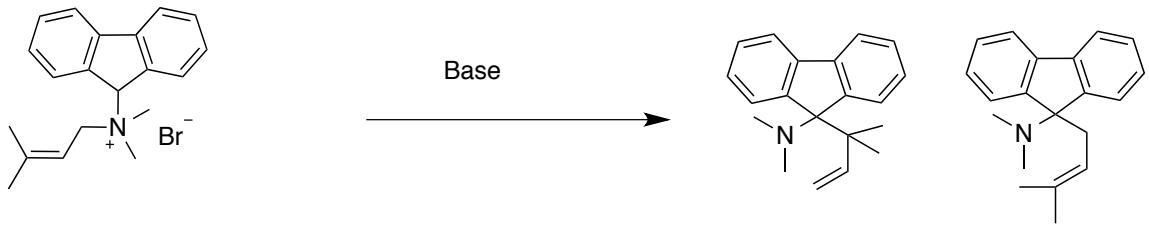
7 **8** **9**

We decided to study DBU mediated rearrangement of the ammonium salt (**7**). When we treated **7** with DBU in acetonitrile at room temperature it gave a mixture of products **8** and **9** and the ratio was found to be approximately 3:4 by ^{1}H-NMR analysis. However, **8** and **9** are inseparable by common analytical techniques. For this reason, we anticipated that **7** might not be suitable for further mechanistic study.

According to the reported literature, when **10** was treated with a base, it afforded a mixture of **11** ([2,3]-product) and **12** ([1,2]-product).[50] For this reason, we sought to study base mediated rearrangement of **10**. When we treated **10** with DBU in acetonitrile at room temperature, it gave a mixture of products **11** and **12**. The ratio was found to be 5:4 by ^{1}H-NMR analysis. In order to evaluate temperature dependence of product ratios

of base mediated rearrangement of **10**, we treated **10** with DBU at -78 °C. The ratio of **11** to **12** was found to be 11:7. Even though the effect of temperature was not profound, lower temperature was found to favor the [2,3]-rearrangement. This is in agreement with common observation regarding temperature dependence of the [2,3]- and [1,2]-product distribution.

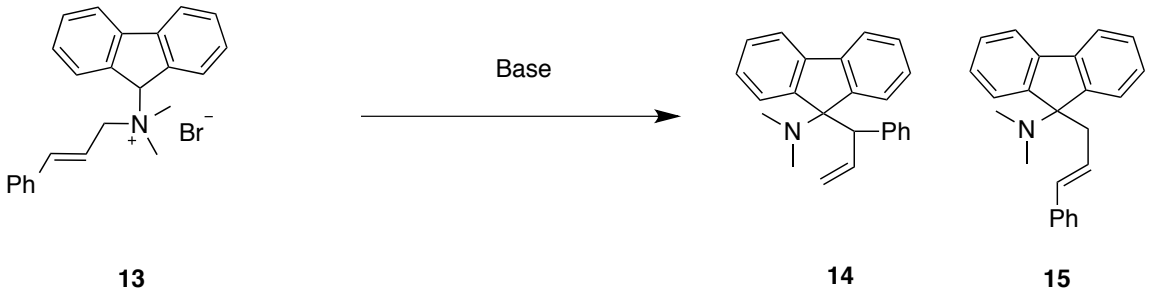
Scheme 4-4



10 **11** **12**

The next system we studied was **13**, which is structurally similar to **10**. We decided to study the system because **13** has been known to give a mixture of **14** ([2,3]-product) and **15** ([1,2]-product) when treated with a base.[50] When reacted with DBU at 25 °C, **13** afforded **14** and **15** in the ratio 5:1. Further we investigated the temperature dependence of the product ratio by carrying out DBU-mediated rearrangement of **13** at 50 °C and at -78°C. At 50 °C the ratio was found to be 4:1 while at -78°C the amount of the [1,2]-product was negligible. The product distribution at different temperatures showed lower temperatures favored the [2,3]-product over the [1,2]-product.

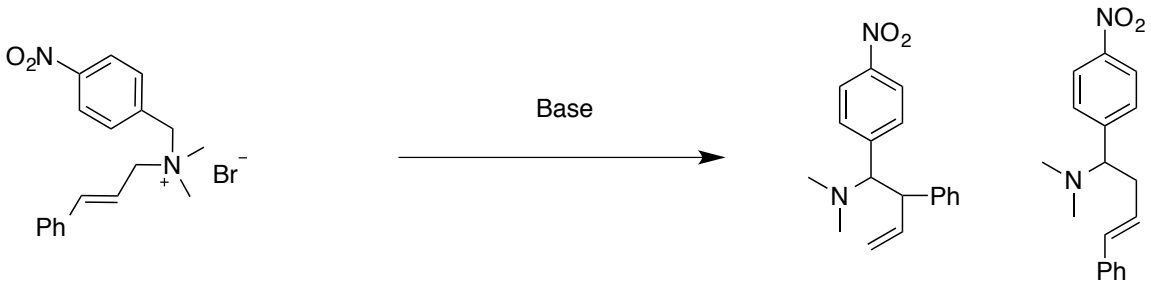
Scheme 4-5



13 **14** **15**

We continued our substrate screening by studying another ammonium salt **16**, which has been known to undergo base mediated rearrangement affording a mixture of the [2,3]- and the [1,2]-products.[36] When we treated **16** with DBU at 25 °C it gave a mixture of **17 (**[2,3]-product) and **18 (**[1,2]-product**)** in the ratio 3:1.

Scheme 4-6

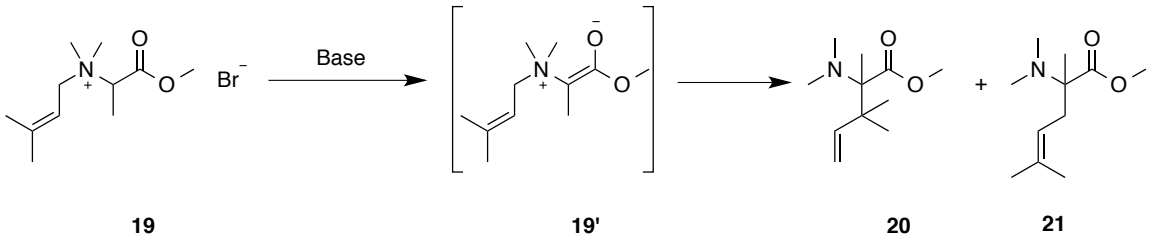


16 **17** **18**

Even though **10**, **13** and **16** afforded a mixture of the [2,3]- and the [1,2]-products when treated with DBU, these systems were structurally very different from the system on which KIEs had been measured. We envisioned that this structural difference might complicate our subsequent mechanistic study. For this reason, we sought to continue our substrate screening to find an ammonium salt which not only gave a mixture of the [2,3]- and the [1,2]-products but was also structurally similar to the system on which KIEs were measured.

In the literature, we found that the ammonium salt (**19**) underwent base mediated sigmatropic rearrangement to afford products **20** ([2,3]-product) and **21** ([1,2]-product) (Scheme 4-7).[36] This system was structurally similar to the system on which KIEs were measured.

Scheme 4-7



Encouraged by the reported result we explored the base mediated rearrangement of **19** by treating it with DBU. We found that when treated with DBU, **19** afforded both

20 ([2,3]-product) and **21** ([1,2]-product). Since **19** gave a mixture of products, we decided to carry out a detailed study of this system. First, we evaluated the temperature dependence of product distribution for the DBU-mediated rearrangement of **19** (Table 4-1). These results suggest that higher temperatures favored the entropically favored dissociation process over the concerted process. Hence, the extent of the [1,2]-product increased.

Table 4-1. Product distribution on DBU-mediated rearrangement of **19**

Temperature	% of 20 ([2,3])	% of 21 ([1,2])
90	80.6	19.4
70	85.3	14.7
50	88.9	11.1
25	95	5

Even though we found that **19** gave a mixture of the [2,3]- and the [1,2]-product we had to consider the possibility of formation of **21** by thermal rearrangement of **20** as it was reported that when **20** was heated to 120 °C it rearranged to **21**.[116] In order to investigate this possibility, we heated a 95:5 mixture of **20** and **21** at 90 °C in acetonitrile for 20 h. However, ^{1}H-NMR analysis of the mixture revealed that the ratio of **20** to **21** did not change by 20 h of heating. This experiment ruled out the possibility of formation of **21** from **20** by thermal rearrangement.

After confirming that **21** had been produced directly from the ylide, **19′** we sought to address another underlying mechanistic possibility. Since the concerted [1,2]-rearrangement is forbidden it is suggested that **21** is formed via the recombination of the diradical **R** (Path-B, Figure 4-2.). However, if the recombination occurs via Path-A, **20** will be formed. So theoretically formation of **20** is also possible via the cleavage path.

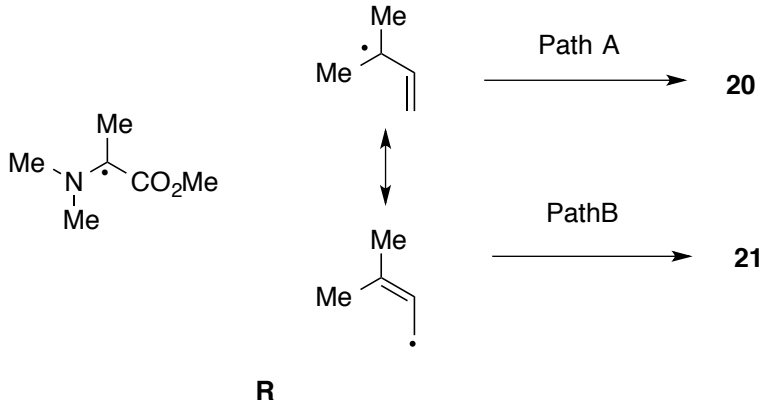
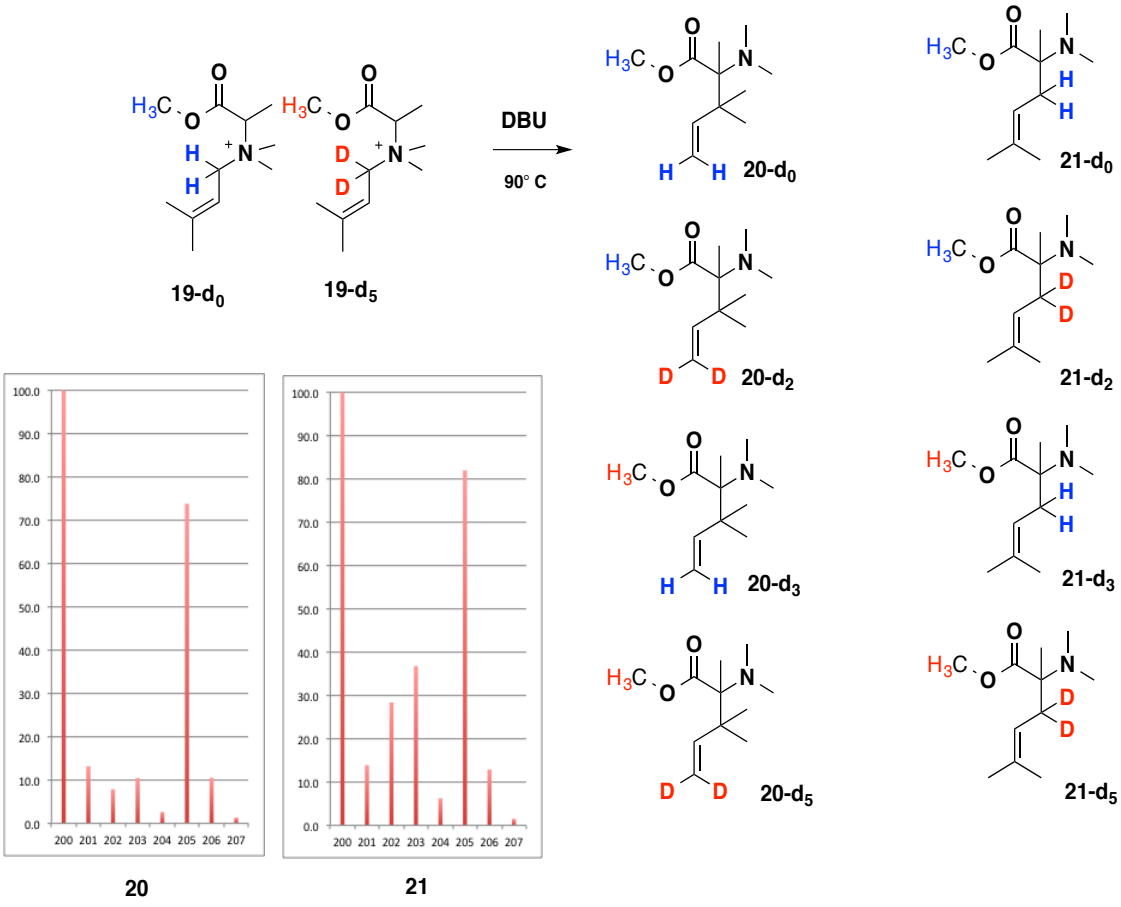


Figure 4-2. Mechanism of formation of **20** and **21** from the diradical **R**

This possibility implied that the product ratio might not be a true reflection of the relative extent of the concerted and the cleavage path. In order to achieve an accurate estimate of the extent of the cleavage, a crossover experiment was carried out at 90 °C with an equimolar mixture of **19** and **19-d_5** (Scheme 4-8). The [2,3]- and [1,2]-products were purified and analysed by ESI-MS. Both **20** and **21** had peaks at M+2 and M+3 indicative of crossover (Scheme 4-8). This result suggested that at least a part of **20** was formed by the cleavage/recombination mechanism.

Scheme 4-8



However, the extent of crossover in the [2,3]-product was found to be 9% while in the [1,2]-product, it was 26%. Low crossover in both the products indicated that the reaction mostly occured by an intramolecular pathway. Importantly, the extent of crossover was higher in the case of the [1,2]-product compared to the [2,3]-product. This observation indicated that the [2,3]-product could be formed by an intramolecular process, that was not available for the [1,2]-product, possibly a concerted rearrangement.

As crossover was observed at 90 °C, we sought to get a more accurate estimate of the extent of cleavage at different temperatures. We performed a similar crossover experiment at 25 °C. ESI-MS analysis was carried out only on the purified [2,3]-product isolated from the crossover experiment as the [1,2]-product could not be purified due to its low proportion (5%) in the reaction mixture. The ESI-MS analysis showed 12% crossover in the [2,3]-product. That result suggested that with decrease in temperature the extent of dissociation of the ylide increases. That meant lower temperature favored the entropically favored path over the enthalpically favored path. Since this experimental observation was not in agreement with the laws of thermodynamics we decided to investigate the origin of this observation. First we established a relationship between the percent conversion of the starting material to the product and the extent of crossover. The analysis of ESI-MS showed that the extent of crossover was not dependent on the extent of conversion of the starting material. This result ruled out the possibility of regeneration of the ylide from the germinate diradicals. We then envisioned that transesterification might be interfering with our experimental results. In order to investigate the effect of transesterification, an equimolar mixture of glycineallylammonium bromide-d_5 (Figure 4-3.) and **19** was subjected to DBU-mediated rearrangement.

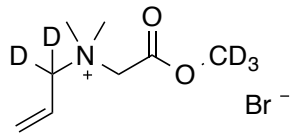
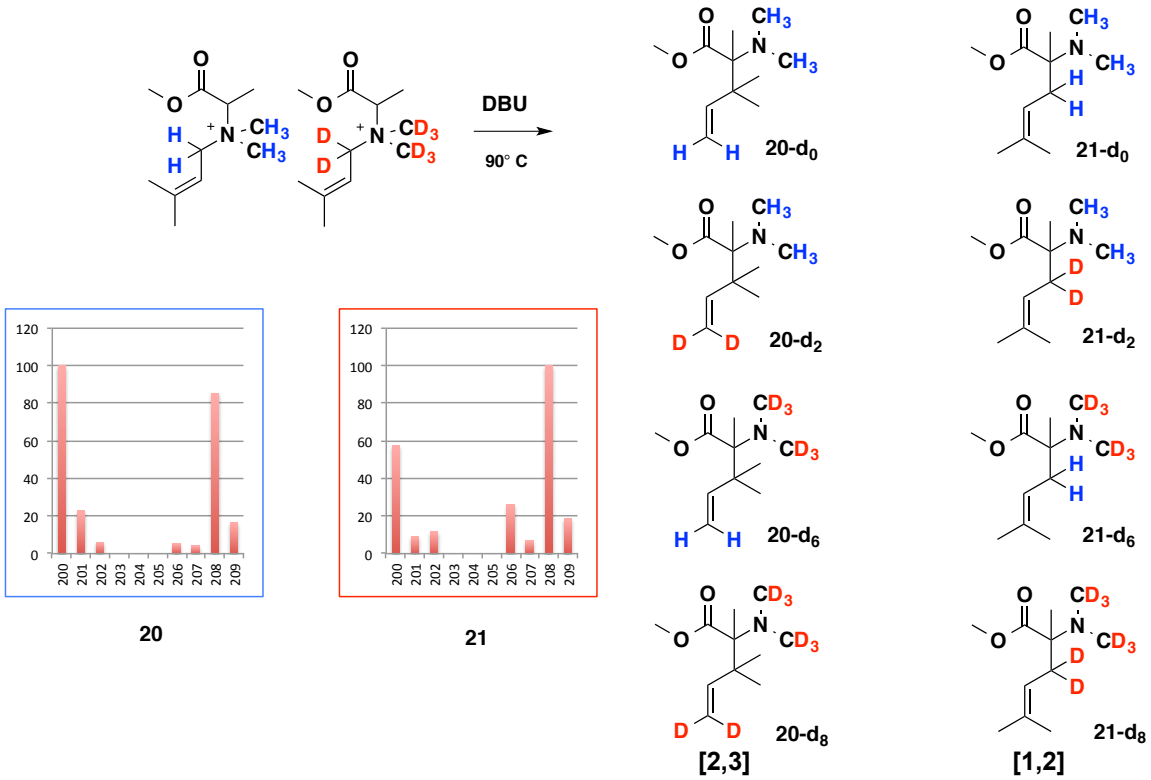


Figure 4-3. Glycineallylammonium bromide-d_5

ESI-analysis of the reaction mixture showed a peak corresponding to **20-d_3** or **21-d_3** (m/z=203). However no peak corresponding to the crossover product was detected. The peak at m/z=203 might be due to the formation of either **20-d_3** or **21-d_3**. This suggested that the results of the crossover experiment with **19-d_5** might be compromised by transesterification. For this reason, we sought to synthesize another isotopically labeled **19** where the crossover result would not be compromised by any side reaction. We anticipated that a crossover experiment with **19-d_8** should not be susceptible towards any side reaction (Scheme 4-9). For this reason, a crossover experiment was performed with an equimolar mixture of **19** and **19-d_8** at 90 °C (Scheme 4-9). The [2,3]- and [1,2]-products were purified and analysed by ESI-MS (Scheme 4-9).

Scheme 4-9



Both **20** and **21** had peaks at M+2 and M+6 indicative of crossover. The extent of crossover in the [2,3]-product was 4.9% while in the [1,2]-product it was 17.9%. That result qualitatively matched with the result obtained with **19-d$_5$**. However, considerable amount of transesterification might be associated with the DBU-mediated rearrangement of **19** as the extent of crossover with **19-d$_8$** was appreciably less compared to the crossover experiment with **19-d$_5$**. In order to get a more accurate estimate of the extent of cleavage path, a crossover experiment with an equimolar mixture of **19** and **19-d$_8$** was carried out at room temperature. The purified [2,3]-product was analyzed by ESI-MS.

The analysis revealed negligible crossover at room temperature. This result suggested that with **19-d_8** there was no appreciable side reaction that could interfere with the result of the crossover experiment.

However, crossover was found in both the [2,3]- and the [1,2]-product (at 90 °C) we inferred that the extent of cleavage was more than the extent of formation of the [1,2]-product. In order to achieve more accurate determination of the extent of cleavage the following kinetic model has been proposed to simulate experimental observations.

Simulation of the Crossover Results with a Kinetic Model

The experimental observables are the extent of formation of **20** (80.4%) and **21** (19.6%), the extent of crossover in **20** (4.9%), in **21**(17.94%) and the ratio of **19** to **19-d_8** (56:44). These values would be predicted by a mathematical simulation on an Excel™ spreadsheet using as variables **x**, **y**, and **z** based on the proposed kinetic model. Here **x** is the fraction of ylide that undergoes concerted process giving only **20**, **y** is the fraction of diradicals formed by cleavage that diffused apart and **z** is the constant fraction of the diffused diradicals that combine to give **20**. The scheme of the kinetic model is shown in Figure 4-4.

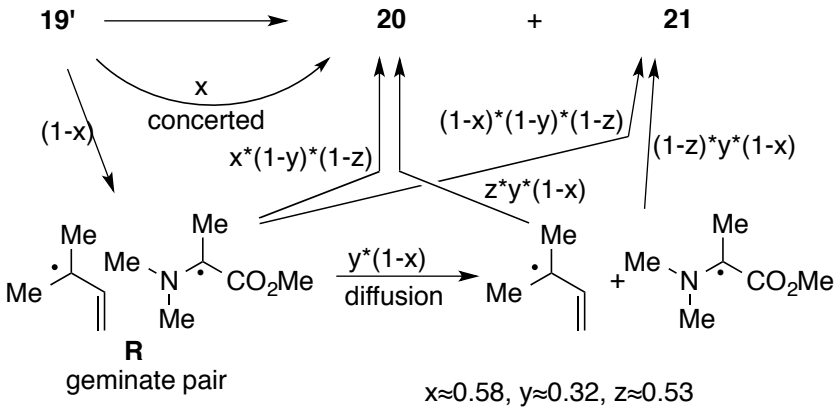


Figure 4-4. Proposed kinetic model for the rearrangement of **19′**

The following equations decides the simulation based on the proposed kinetic model:

20-d_0: = A6*A4 + A4*B6*B8*A10 + A4*B6*A8*A10*A4

20-d_2: = B4*B6*A8*A10*A4

20-d_6: = B4*B6*A8*A10*A4

20-d_8: = A6*B4 + B4*B6*B8*A10 + B4*B6*A8*A10*B4

21-d_0: = A4*B6*B8*B10 + A4*B6*A8*B10*A4

21-d_2: = B4*B6*A8*B10*A4

21-d_6: = B4*B6*A8*B10*A4

21-d_8: = B4*B6*B8*B10 + B4*B6*A8*B10*B4

where

A4 is the fraction of **19** versus **19**-d_8 (0.56), B4 = 1-A4

A6 = **x**, B6 = 1-**x**

A8 = **y**, B8 = 1-**y**,

A10 = **z**, B10 = 1-**z**

The fraction of the [2,3]-product **20** was then just determined by (**20-d_0** + **20-d_2** + **20-d_6** + **20-d_8**) / (**20-d_0** + **20-d_2** + **20-d_6** + **20-d_8** + **21-d_0** + **21-d_2** + **21-d_6** +**21-d_8**) The fraction of crossover in **20** was calculated as **20-d_6** / (**20-d_6** + **20-d_8**). The fraction of crossover in **21** was calculated as **21-d_6** / (**21-d_6** + **21-d_8**).

The solver function in Excel™ was then employed for minimizing the difference between the experimental and model-predicted values. Numerical solution leads to values of **x**=0.58, **y**=0.32 and **z**=0.53. However, an analytical solution of these equations is also possible as there are three variables and three equations.

It is important to consider the sources of possible errors in the result due to the limitations of the kinetic model. Firstly, it is possible that the germinate radicals that diffused might not recombine together to form the sigmatropic rearranged products. Exclusion of this effect would underestimate the extent of cleavage. However we were not able to identify any species that could be products of the side reactions associated with those germinate radicals. This could be due to the "persistent radical effect", side products formation via radical-radical recombination is negligible. However, it is logical to believe that we were unable to identify small amount of side products in the reaction mixture. In order to address the effect of the unidentifiable side products from radical-radical recombination, the simulation was done with the assumption that only 50% of the diffused radicals form either **20** or **21**. Inclusion of this assumption changed the values of **x**, **y**, and **z** to 0.516, 0.485, and 0.528, respectively. This clearly showed that inclusion of this assumption decreases in the extent of concerted process. Secondly, an error could be associated with the assumption in the model that a definite fraction **z** of the recombining

radicals give **20**, regardless of whether recombination occurs from the initial geminate pair or after diffusion. It is quite possible that the geminate radical pair is created in such a way that there is a preference for formation of **20** over **21**. This preference is most likely to be governed by the relative orientation of the combining radicals. Considering the possible errors associated with simulation of the kinetic model it could be inferred that the kinetic model overestimated the extent of the concerted path. Thus the value of **x**= 0.58 should rightly be described as the upper limit of the concerted path. Finally, we confirmed non-involvement of DBU, by treating **19** with KH at 25 °C. The ratio of **20** to **21** was found to be same as with DBU. As experimentally we were able to get fairly good estimation of the extent of the cleavage path we decided to carry out theoretical calculations for in depth mechanistic study of the rearrangement of **19′**.

Theoretical Study and Discussions

In order to understand the experimental observations, we sought to study the base-mediated rearrangement of **19** via theoretical calculations. First, we located four [2,3]-rearrangement TSs (from **TS1** to **TS4**, Figure 4-5).

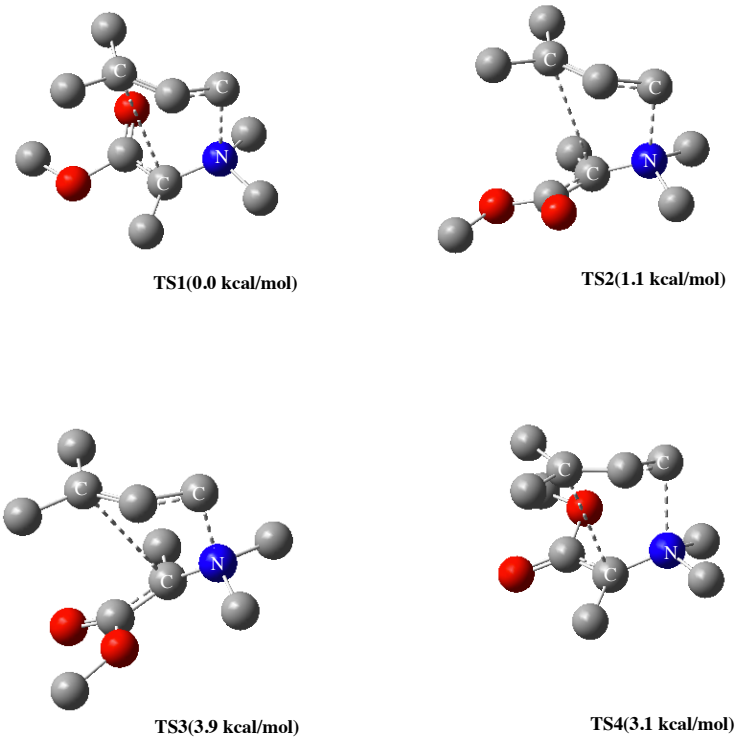
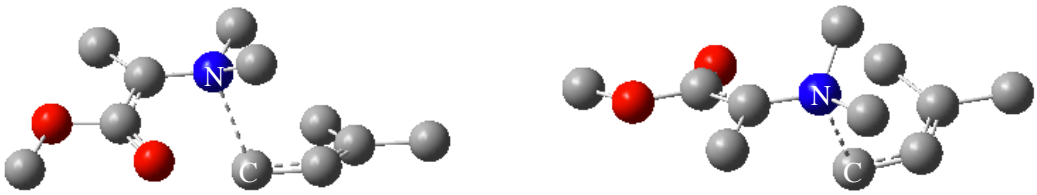


Figure 4-5. Four TSs of the [2,3]-rearrangement of **19′** (all H-atoms were omitted for clarity)

In case of B3LYP/6-31G*/Gas-Phase, **TS1** is the lowest energy TS and it is 1.1 kcal/mol lower in free energy than the next higher energy TS (**TS2**). The contribution of other two TSs (TS3 and TS4) should be negligible as those are 3-4 kcal/mol higher in energy. The relative energies of the TSs were also checked with other methods (M062X, M06, O3LYP). Regardless of the method used, **TS1** was the lowest energy TS. In this dissertation, all the subsequent calculations have been performed on the lowest energy TS (**TS1**).

Variational TST Rates for the C-N Bond Cleavage versus the [2,3]-Rearrangement

Traditionally it has been suggested that the relative ratio of the concerted path and cleavage path depends on the free energy difference between the TSs of the two paths. For this reason, we decided to examine the validity of the traditional explanation by calculating the free energies of the TSs of the two paths. Since the cleavage path has an entropic advantage over the concerted path, an accurate evaluation of the free energies of the TSs was required. Two TSs were located for cleavage path (**TS′1** and **TS′2** Figure 4-6.).



TS'1(0.0kcal/mol) **TS'2(0.8 kcal/mol)**

Figure 4-6. Two TSs of C-N cleavage of **19′** [B3LYP/6-31G*/PCM (CH_3CN)] (all H-atoms were omitted for clarity)

Even though the difference in energy between two TSs was close we chose to carry out subsequent calculations with the lowest energy TS (**TS′1**) because in case of concerted path similarly the second lowest TS (**TS2**) is also only 1.1 kcal/mol higher in energy than the lowest energy TS (**TS1**) and the contribution of **TS2** was ignored.

The free energy calculations were carried out on UB3LYP-D2, UM06, and UM06-2X energy surfaces, each employing a 6-31+G** basis set including a PCM solvent model for acetonitrile. As the effect of entropy at the TS might be significant the TSs located on the potential energy surface may not accurately represent the TS for the process. In order to carry out more accurate calculations, GAUSSRATE calculations were employed. Importantly, the conformations of the starting materials in GAUSSRATE calculations for concerted and cleavage processes should be different. To compare rate constants accurately, we allowed for the difference in free energies of the starting materials at the temperature of interest, 90 °C. The outcomes of the calculations are summarized in Table 4-2.

Table 4-2. Relative rate constants for C-N bond cleavage versus [2,3]-rearrangement

Method[a]	**Rate constants (s^{-1})**		**Raw ratio of rate constants**[c]	**Free energy difference of starting material (kcal/mol)** [c, d]	**Corrected ratio of rate constants**[c]
	[2,3]-rearrangement[b, c]	**Cleavage**[b, c]			
(U) M06	3.69E+05	5.02E+03	73.5	0.467	38.5
(U) M062X	2.56E+01	1.49E+00	17.2	-0.731	47.3
(U) B3LYP-D2	8.18E+06	5.78E+05	14.2	-0.4	24.6

[a]The calculation was done by 6-31+G**/PCM. [b]The rate constants are CVT/SCT rate constants. [c]The temperature was 90 °C. [d]The difference is defined as the energy of the [2,3]-rearrangement starting material compared to cleavage starting material.

In all cases, the GAUSSRATE calculations suggested that the extent of cleavage should not be more than 2-4%, which was at least 15 times lower than the lower limit of the experimentally observed extent of cleavage. These results clearly indicated that the relative free energy of the TSs of the competing concerted and cleavage path could not account for the extent of cleavage for base mediated rearrangement of **19**.

Even though the GAUSSRATE calculations clearly indicated the relative free energy of the TSs of cleavage and concerted path could not account for experimental results, we questioned the reliability of the DFT methods. In order to detect any systematic error, we sought to compare the DFT results with high level ab initio calculations.

Exploration of Ab Inito Methods

Before employing high level calculations, we even wanted to investigate the relaibility of those methods by comparing the predictions by those methods with experimental results. In order to check their reliability, we computed the dissociation of the C-H bond in ethane and the central carbon-carbon bond of 1,5-hexadiene using UBD(T) method. When the basis set was considerably small, the method failed (e.g. 6-31G*, cc-pvdz) to predict successfully experimental results. It actually underestimated the barriers for these dissociations. However, medium-sized basis sets (e.g. 6-311+G**, augcc- pvdz) worked considerably well. The mentioned dissociations were further investigated by even larger basis-set cc-pvtz. As we increased the size of the basis set, the extent of accuracy of the prediction the experimental results increased. That

observations indicated reliability of that high level calculations.

However, when we tried to employ UBD(T) method to detect systematic errors in DFT calculations, we faced two obstacles. Firstly, the experimental system is too large even for single point energy calculations by UBD(T). For this reason, we decided to employ model systems **A** and **B** that would mimic the experimentally studied system (Figure 4-7).

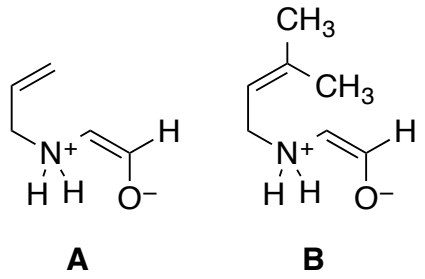


Figure 4-7. Model systems chosen for high level calculations

Secondly, even with the model systems the employment of large basis-sets is impractical. Considering the effects of basis-sets on accuracy of calculations we decided to use medium sized basis-sets (6-31+G* and 6-311+G**). After deciding on the model systems and basis-sets we sought to explore the energy difference between the TSs of concerted (rearrangement) path and cleavage path on model systems **A** and **B**. It was not possible to locate TSs by UBD(T) method. So we decided to locate the TSs by a suitable DFT-method and then calculated the energy of the located TS by that high level ab initio

method. We decided to use (U)M06/6-31+G**(gas phase) to locate the TSs. After locating the TSs, we calculated the energy of the single point by different DFT-methods and (U)BDT methods to locate the direction of the error associated with DFT calculations.

Table 4-3 summarized the results obtained from single point energy calculations. The first column provides descriptions of the system and nature of the single point, whether it is starting material (**A** or **B**), rearrangement TS or cleavage TS. The second column represents the method, basis-set and absolute energy of the corresponding species. The third column provides information about the potential energy barrier for the rearrangement and cleavage process (in kcal/mol). The fourth column represents the relative energy of the cleavage TS compared to the rearrangement TS. The last column is designated as "Bias for cleavage". This information of this column was defined by comparing the relative barrier for the cleavage TS versus the rearrangement TS calculated by the DFT methods versus those calculated by the UBD(T) methods with a cc-pvtz basis set for system **A** and aug-cc-pvdz basis set for system **B**. The positive values in this column would suggest that the DFT calculation underestimated the barrier for cleavage process while negative values would suggest that particular DFT-method overestimated the barrier of the cleavage path. On analyzing these values it is quite clear that regardless of the choice of the method used DFT-methods favored the cleavage path compared to (U)BDT. The extent of favor varied widely depending on the choice of methods and basis-sets.

Table 4-3. UBDT and DFT methods for [2,3]-rearrangement and bond cleavage

Structure	Method	P.E. Barrier	Relative Cleavage Barrier	Bias favoring cleavage
	UBD(T)/6-31+G**			
A	-324.968154			
[2,3]-TS	-324.944803	14.7		
cleavage ts	-324.927008	25.8	11.2	
	UBD(T)/6-311+G**			
A	-325.086484			
[2,3]-TS	-325.063202	14.6		
cleavage ts	-325.044343	26.4	11.8	
	UBD(T)/aug-cc-pvdz			
A	-325.029883			
[2,3]-TS	-325.008653	13.3		
cleavage ts	-324.988515	26.0	12.6	
	UBD(T)/cc-pvtz			
A	-325.291245			
[2,3]-TS	-325.267234	15.1		
cleavage ts	-325.247319	27.6	12.5	
	DFT methods			
	(U)M06/6-31+G**			
A	-325.637319			
[2,3]-TS	-325.616474	13.1		
cleavage ts	-325.603027	21.5	8.4	4.1
	(U)M062X/6-31+G**			
A	-325.706939			
[2,3]-TS	-325.681698	15.8		
cleavage ts	-325.664881	26.4	10.6	1.9
	(U)B3LYP/6-31+G**			
A	-325.868930			
[2,3]-TS	-325.851119	11.2		
cleavage ts	-325.842746	16.4	5.3	7.2
	(U)B3LYP/6-31+G**/D2			
A	-325.882674			
[2,3]-TS	-325.869143	8.5		
cleavage ts	-325.856733	16.3	7.8	4.7

Table 4-3. Continued

Structure	Method	P.E. Barrier	Relative Cleavage Barrier	Bias favoring cleavage
	UBD(T)/6-31+G**			
B	-403.377433			
[2,3]-TS	-403.352115	15.9		
cleavage ts	-403.335068	26.6	10.7	
	UBD(T)/6-311+G**			
B	-403.522106			
[2,3]-TS	-403.496345	16.2		
cleavage ts	-403.478526	27.3	11.2	
	UBD(T)/aug-cc-pvdz			
B	-403.450655			
[2,3]-TS	-403.427451	14.6		
cleavage ts	-403.407668	27.0	12.4	
	DFT methods			
	(U)M06/6-31+G**			
B	-404.216812			
[2,3]-TS	-404.194027	14.3		
cleavage ts	-404.181690	22.0	7.7	4.7
	(U)M062X/6-31+G**			
B	-404.308210			
[2,3]-TS	-404.279571	18.0		
cleavage ts	-404.264754	27.3	9.3	3.1
	(U)B3LYP/6-31+G**			
B	-404.512971			
[2,3]-TS	-404.491524	13.5		
cleavage ts	-404.486286	16.7	3.3	9.1
	(U)B3LYP/6-31+G**/D2			
B	-404.536481			
[2,3]-TS	-404.521091	9.7		
cleavage ts	-404.509314	17.0	7.4	5.0

From the last column it is evident that the favor for cleavage was least for M062X method and highest for B3LYP method. This comparison suggested that higher

level calculations would likely predict even lesser extent of cleavage compared to DFT-methods based on the energy difference of the two TSs for the experimental system.

Molecular Dynamics

Our theoretical calculations based on TST and variational transion state theory (VTST) revealed that the relative energy of the rearrangement and cleavage TSs could not account for the experimentally observed extent of the cleavage process. Based on our theoretical results and experimental observations, we inferred that the free energies of the TSs could not be responsible for such competition. Since energetics failed to account for the extent of cleavage, we hypothesized that the molecular motions and molecular momenta could be responsible for such competition. In order to investigate our hypothesis, we decided to run dynamic trajectories on the TS of the [2,3]-rearrangment.

Outcome of Molecular Dynamics Calculations

Dynamic trajectories were carried out from the area of the saddle point region in the potential energy surface of the [2,3]-rearrangment. It was found that there are dynamic trajectories that formed **20**. The formation of **20** confirmed that the located TS is indeed a TS for [2,3]-rearrangment. However not all trajectories formed **20**, interestingly, an appreciable portion of the trajectories formed diradical, **R** . These radicals can recombine to give both the [1,2]- and the [2,3]-products. The results of the calculations using different methods have been summarized in Table 4-4. Regardless of the method used, a portion of the trajectories formed the diradical **R**. However, with

(U)M062X TS, the extent of diradical formation is least which could be understood from the fact that M062X calculation located the tighest TS among all the theoretical methods used. On the other hand, the loosest TS located by M06 calculation provided highest extent of cleavage.Even though a part of dynamic trajectories from the TSs of all methods led to dissociation it is important to mention that none of the predicted ratios of rearrangement and cleavage perfectly matched the experimental ratio. However, considering the limitations of the computed unrestricted energy surfaces and the lower-limit nature of the experimentally observed extent of cleavage we infer here that the theoretical predictions were in good agreement with the experimental observation. A qualitative understanding of the cleavage process from **TS1** is going to be discussed in the next paragraph.

Table 4-4. Outcome of trajectories passing through TS1

Method/Basis Set/Solvent Model	**Rearrangement (**20**): Cleavage (**R**)**
UB3LYP-D2/6-31G*/PCM[a,c]	74:111 (40%:60%)
UB3LYP-D2/6-31G*/PCM[b,c]	33:114 (22%:78%)
UM06-2X/6-31G*/PCM[b,c]	319:68 (82%:18%)
UM06-2X/6-31G*/PCM[b,d]	274:35 (89%:11%)
UM06-2X/6-31+G**/PCM[b,c]	64:22 (74%:26%)
UM06/6-31G*/PCM[b,c]	9:79 (11%:89)
ONIOM with 24 CH_3 [a,c,e]	32:44 (42%:58%)
experimental	58%:42% (upper limit)

[a]Fully classical. [b]Quasiclassical.. [c]90 °C. [d]25 °C. [e]The ONIOM used UB3LYP-D2/6-31G* for the atoms of **TS1** and PM3 for the CH3CN molecules. The trajectories were started from a transition structure located after a series of cycles of simulated annealing.

Considering dynamical point of view, the cleavage process could be understood with reference to the overlays of trajectory points in the following figure (Figure 4-8). At the transition state the C^3−N bond is breaking and this process continues as the time passes. During that time if C^1 and C^5 approach each other the trajectory will end up giving the [2,3]-rearrangement product (**20**).

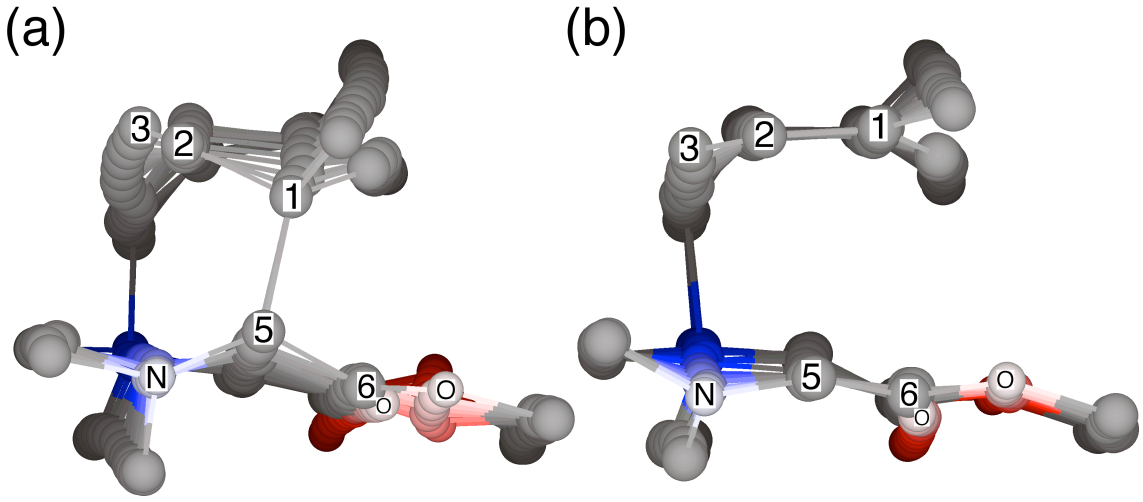


Figure 4-8. Overlays of trajectory points. (a) a concerted [2,3]-rearrangement, and (b) simple cleavage, with both occurring through the same transition state. The points are spaced at 10-fs intervals. Earlier points are darker and in back. The transition state is about one-third from the back

However, at the transition state the interaction between C^1 and C^5 is not strong, and motions along the orthogonal modes can surpass the motion in the direction of the transition vector. When this motion along the orthogonal modes nullifies the effect of the motion leading to approach of C^1 and C^5, cleavage occurs. However, in case of trajectories that zeroed out the energies in orthogonal modes, ended up to **20**, regardless of the energy of the transition vector. When classical trajectories were carried out instead of quasiclassical trajectories the extent of cleavage slightly decreased.

In order to investigate the effect of solvent molecules towards the experimental outcome dynamic trajectories were carried out with explicit solvent (acetonitrile) molecules. However, the predicted extent of cleavage with explicit solvent molecules did not differ appreciably from the results with implicit solvent model. This could be

understood from the fact that the solvents rarely collide with the reaction species during the course of rearrangement.

From a statistical point of view, the formation of both the [2,3]-rearranged product and the diradical from a single transition state could be viewed as a bifurcation in the free-energy surface. The [2,3]-rearrangement is downhill enthalpically from the transition state, but it is entropically disfavored as new bond formation is associated with a constriction of motion. When the reaction was studied by VTST calculations there were no additional dynamic bottlenecks for formation of **20**. Since the formation of **20** and **R** is comparable in the trajectories, we could logically assume that there is no barrier in free energy surface to form **R** from the [2,3]-rarrangment TS. The formation of **R** is indeed enthalpically disfavored over the rearrangment process that leads to **20**, because during this process one bond breaks and no new bond is formed. However formation of **R** has an entropic advantage because two species are formed from one species via the cleavage of one bond.

Even though cleavage could occur from **TS1** one could raise a question about the origin of facility of bond cleavage via **TS1** over **TS′1**. This is because the C^3–N bond cleavage via **TS′1** or bond cleavage via **TS1** is essentially associated the same overall thermodynamic demand. The facility of cleavage via **TS1** over **TS′1** could be explained by considering Figure 4-8. In this figure the thermodynamic course of cleavage via **TS1** and **TS′1** has been depicted.

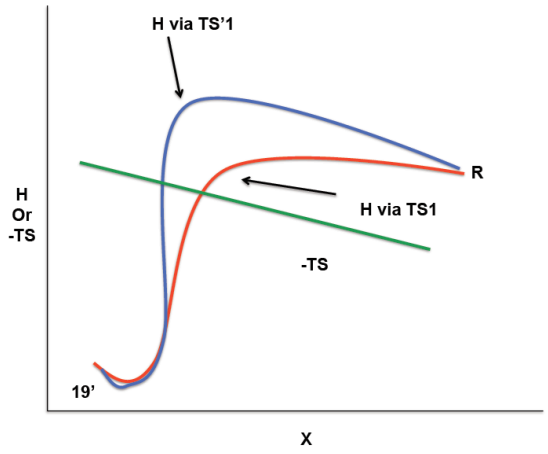


Figure 4-9. Qualitative reaction coordinate diagram. This diagram is illustrating the advantage of forming **R** via **TS1** over **TS′1**. Cleavage becomes barrierless in G when the drop in –TS exceeds the rise in H

At the VTS, Gibbs free energy, G is maximum. Therefore at VTS the slope of the Gibbs free energy of the reacting system is zero. So at the VTS the slope of enthalpy will be equal to the slope of entropy multiplied by absolute temperature (equation 4-1).

$$(dH/dX)_T = T*(dS/dX)_T \qquad (4\text{-}1)$$

Now considering the Figure 4-8 and equation 4-1 it is quite clear that the cleavage via the [2,3]-rearrangement TS is associated with lower free energy barrier.

In qualitative terms, the cleavage via rearrangement TS is stabilized by a pericyclic orbital interaction that allows the process less enthalpically demanding. As cleavage continues the free energy drops due to increase in entropy. As a result, the free-energy barrier for cleavage is lowest along the path through the rearrangement TS (**TS1**).

Even though our hypothesis was supported by the outcome of dynamic trajectory calculations it is important to discuss some technical issues that were encountered while carrying out dynamic trajectories. Discussions of these technical issues are important to judge the reliability of our trajectory calculations. These issues will be discussed in the next two sections.

Stability of the Wavefunction

Dynamic trajectory calculations were carried out under unrestricted method and "guess=mix" keyword was used in Gaussian09. However, guess=mix is not fully reliable, and there are occasions where this option failed, leading to complication associated with wave function instability. In trajectories that lead to bond cleavage, that is, after the C^3-N distance is greater than 2.9 Å and with the C^1-C^5 distance > 3.2 Å, guess=mix option could not always lead to the broken-symmetry solution. This was recognized by the presence of points in the trajectories having S^2=0 in the midst high S^2 values. Those geometries were checked with the "stable=opt" option in Gaussian09. This option led to a lower energy broken symmetry solution. However, those points did not have any effect on the outcome of the trajectory calculations. Since from those bad points the fragmented parts never recombined. The trajectories which led to rearrangement never showed any contribution of such points.

Effect of Spin-Contamination

As the cleavage is homolytic in nature the effect of spin contamination was

carefully examined. To examine the range of geometries that might subject to spin contamination, exploratory studies of grids of geometries associated with bond cleavage in **19′** were carried out in two different methods (M06-2X/6-31G* and M06/6-31G*). It was found that S^2=0 when breaking C^3-N < 2.3 and forming C^1-C^5 < 3.4, and when C^3-N < 2.4 and C^1-C^5 < 3.0, and when C^3-N < 2.5 and C^1-C^5 < 3.9, and when C^3-N < 2.6 and C^1-C^5 < 2.8, and when C^3-N < 2.7 and C^1-C^5 < 2.7. If the bond distance exceeds the mentioned ranges, significant spin contamination has been observed.

After checking the B3LYP, M06-2X, and M06 [2,3]-rearrangement transition structures with the "stable=opt" option in Gaussian09, and many of the [2,3]-rearrangement transition structure with the guess=mix option we concluded that the for rearrangement process is devoid of any spin contamination. In all cases, the 2,3-rearrangement transition structures had a stable S^2=0 wavefunction. The cleavage transition states **TS′1** exhibited spin contamination with S^2 values before annihilation of 0.37 to 0.54. As shown by the comparison of model DFT versus UBD(T) energetics described before, the error in these structures likely underestimates their energy.

We noted that the surfaces for cleavage via the [2,3]-rearrangement transition state **TS1** and direct cleavage via **TS′1** were both subject to the same spin contamination error, and it seems fair to expect some cancellation of error in the comparison of bond cleavage via **TS1** with that via **TS′1**.

Conclusion

We believe, the study discussed in the chapter answered a very fundamental

mechanistic question that was not answered previously. The ammonium ylide (**19′**) that was studied gives a mixture of the [2,3]- and [1,2]-products. Considering both the extent of formation of **21** and extent of crossover in **20** and **21**, we were able to estimate the lower limit of extent of cleavage. However, both TST and VTST failed to account for the experimentally observed extent of cleavage path.

As energetics failed to account for overwhelming extent of cleavage process we envisioned that molecular motions might be responsible for the cleavage. For this reason dynamic trajectory calculations were carried out from the formal [2,3]-rearrangement TS. We found that there were trajectories that formed **R** from the [2,3]-rearrangement TS. The extent of cleavage predicted by dynamic trajectory calculations was in good agreement with experimentally measured extent of cleavage. We here argue that the allowed pericyclic reaction, [2,3]-rearrangment facilitates the formally forbidden [1,2]-rearrangement.

Certainly, the [1,2]-rearrangement could occur without assistance of the [2,3]-rearrangement TS. There are literature examples where the [2,3]-rearrangement TS is just not sterically feasible but still the [1,2]-rearrangement occurs (Figure 2.12, CHAPTER II). However, literature reports also suggest that loose character of the [2,3]-rearrangement TS is quite common feature.[18] We here propose that from the loose [2,3]-rearrangement TS, cleavage could also occur and this is the cause for common co-occurrence of [2,3]- and [1,2]-sigmatropic rearrangements.

Even though, we were successful to predict the experimental outcome of the allyl ammonium systems we did not explore other systems where competition between the

[2,3]- and [1,2]-rearrangements have been observed. We sought to test our hypothesis to other systems. We decided to extend our study towards benzylic systems where the competition is more prevalent. A mechanistic study on rearrangement of benzyl ammonium ylides has been discussed in the next chapter.

Furthermore, we believe that rational chemical methodology development should rely on deep understanding of reaction mechanisms. However, even today, methodology development heavily relies on previously observed phenomena and qualitative understanding of reactions. This method has been successful yet it requires tremendous amount of experimental efforts. For this reason, we envisioned that theoretical calculations could be employed for methodology development. This should minimize the experimental effort towards methodology development. In the next chapter, we have also discussed our effort to utilize theoretical calculations towards methodology development.

Experimental Procedures

Synthesis and Base-mediated Sigmatropic Rearrangement 1, 4, 7, 10, 13, 16 and 19

Synthesis of N, N-dimethylcinnamylamine

A mixture of 7.2 g (64.00 mmol) of 40% aqueous solution of dimethylamine and 8 mL of acetonitrile was cooled to 0 °C in an ice-bath. After cooling, 1.95 g (12.80 mmol) of cinnamyl chloride was added and the mixture was stirred at 0 °C for 24 h. The

stirring was continued further for 12 h at room temperature. The reaction mixture was then poured into 20 mL of water and the organics were extracted with three 50- mL portions of diethyl ether. The ether extracts were combined and dried over anhydrous potassium carbonate. The ether was then removed on a rotatory evaporator to afford 1.44 g (8.96 mmol, 70%) crude N,N-dimethylcinnamylamine, judged to be more than 95% pure by NMR analysis. ^{1}H NMR spectrum was compared with the previously reported ^{1}H NMR. (CDCl3): δ 2.16 (s, 6 H), 2.95 (d, J = 7.0 Hz, 2 H), 6.15 (m, 2 H), 6.4(d, J = 16.0 Hz, 1 H), 7.20 (m, 5 H). The aromatic peaks overlap with the solvent peak.

Synthesis of 2-(Dimethylamino)-1-phenylpropan-1-one

A mixture of 530 mg (4.70 mmol) of 40% aqueous solution of dimethylamine and 6 mL of acetonitrile was cooled to 0 °C in an ice-bath. After cooling, 415 mg (2.35 mmol) of 2-bromopropiophenone was added and the mixture was stirred at 0 °C for 12 h. The stirring was continued further for 12 h at room temperature. After 12 hours of stirring 10 mL water was added and the reaction mixture was saturated with NH_4Cl. Then the organics were extracted with three 10- mL portions of diethyl ether. The ether extracts were combined and dried over anhydrous sodium sulfate. The volatiles were then removed on a rotatory evaporator to afford 243 g (1.67 mmol, 71%) crude 2-(dimethylamino)-1-phenylpropan-1-one, judged to be more than 95% pure by NMR analysis. ^{1}H NMR spectrum was compared with the previously reported ^{1}H NMR for 2-(dimethylamino)-1-phenylpropan-1-one. (CDCl3): δ 1.26 (d, J = 7.0 Hz 3 H), 2.32 (s, 6 H), 4.07 (q, J = 7.0 Hz, 1 H), 7.50 (m, 3 H), 8.06 (m, 2 H).

Synthesis of N,N-dimethylprenylamine

A mixture of 45.00 g (400 mmol) of 40% aqueous solution of dimethylamine and 8 mL of acetonitrile was cooled to 0 °C in an ice-bath. After cooling, 2.32 g (22.30 mmol) of prenyl chloride was added and was the mixture was stirred at room temperature for 20 h. After 20 h of staring the organics were extracted three 50- mL protions of ether. The ether layer was then washed with 20- mL of water. Then the ether layer was dried over anhydrous sodium sulfate. The volatiles were removed on a rotatory evaporator to afford 1.00 g (8.92 mmol, 40%) of crude N,N-dimethylprenylamine, judged to be more than 95% pure by NMR analysis. ^{1}H NMR for N,N-dimethylprenylamine. (CDCl3): δ 1.61 (s, 3 H), 1.7.0 (s, 3 H), 2.18 (s, 6 H), 2.82 (d, J = 6.5 Hz, 2 H), 5.21(t, J = 6.5 Hz, 1 H).

Synthesis of N,N-Dimethylalanine Methyl Ester

A mixture of 4.50 g (39.55 mmol) of 40% aqueous solution of dimethylamine and 4 mL of acetonitrile was cooled to 0 °C in an ice-bath. After cooling, 3.31 g (19.82 mmol) of methyl 2-bromopropanoate was added and the mixture was stirred at 0 °C for 12 h. The stirring was continued further for 12 h at room temperature. The reaction mixture was then poured into 20 mL of water and the organics extracted with three 50-mL portions of diethyl ether. The ether extracts were combined and dried over anhydrous sodium sulfate. The ether was then removed on a rotatory evaporator to afford 1.00 g (7.53 mmol, 38%) crude N,N-dimethylalanine methyl ester (**1**), judged to be more than 95% pure by NMR analysis. ^{1}H NMR (399.53 MHz, $CDCl_3$): δ 1.27 (d, J =

7.0 Hz, 3 H), 2.31 (s, 6 H), 3.22 (q, J =7.0 Hz 1 H), 3.70 (s, 3 H). ^{13}C NMR (75.42 MHz, $CDCl_3$): δ 14.7, 41.9, 51.6, 63.0, 173.9.

*Synthesis of **1***

To a mixture of 890 mg (7.61 mmol) of NN-dimethylglycine methyl ester and 2 mL of acetonitrile (dried over calcium hydride and distilled under nitrogen) under nitrogen was added 3.00 g (15.22 mmol) of cinnamyl bromide. The resulting mixture was stirred for 12 h. After that 10 mL of ether was added to the reaction mixture. The solid thus precipitated out was washed with twice 10 mL of portions ether affording 1.60 g (5.1 mmol, 67%) of **1**. The ^1H NMR of the solid was analyzed and compared with the previously reported ^1H NMR of **1**. ^1H NMR ($CDCl_3$) δ 3.60 (s, 6 H), 3.77 (s, 3 H), 4.84 (d, J = 8 Hz, 2 H), 5.11(s, 2 H), 6.28 (m, 1 H), 7.07 (d, J = 15.3 Hz, 1 H), 7.38 (m, 3 H), 7.47 (m, 2 H).

*Synthesis of **4***

To a mixture of 100 mg (0.51 mmol) of 2-bromoacetophenone and 2 mL of acetonitrile (dried over calcium hydride and distilled under nitrogen) under nitrogen was added 100 mg (0.62 mmol) of N,N-dimethylcinnamylamine. The resulting mixture was stirred for 12 h. After that 10 mL of ether was added to the reaction mixture. The solid thus precipitated out was washed with twice 10 mL portions of ether affording 141 mg (0.39 mmol, 77%) of **4**. The ^1H NMR of the solid was analyzed and compared with the previously reported ^1H NMR of **4**. ^1H NMR ($CDCl_3$) δ 3.65 (s, 6 H), 4.88 (d, J = 8.5 Hz,

2 H), 5.87 (s, 2 H), 6.29 (m, 1 H), 7.07 (d, J = 15.3 Hz, 1 H), 7.30-7.68 (m, 8 H), 8.12 (d, J=7.9, 2 H).

*Synthesis of **7***

To a mixture of 300 mg (1.70 mmol) of 2-(dimethylamino)-1-phenylpropan-1-one and 5 mL of ether (dried over calcium hydride and distilled under nitrogen) under nitrogen was added 250 mg (1.70 mmol) of prenyl bromide. The resulting mixture was stirred for 12 h. The solid thus precipitated out was washed with five times 10 mL portions of ether affording 380 mg (1.17 mmol, 69%) of **7**. The ^{1}H NMR of the solid was analyzed and compared with the previously reported ^{1}H NMR of **7**. ^{1}H NMR ($CDCl_3$): δ 1.75 (d, J=7.1 Hz, 3 H), 1.84 (s, 3 H), 1.85 (s, 3 H), 3.41 (s, 3 H), 3.50 (s, 3 H), 4.35 (dd, J = 8.4 Hz, 12.6 Hz, 1 H), 4.60 (dd, J = 8.4 Hz, 12.6 Hz, 1 H), 5.47 (t, J = 8.4 Hz, 1 H), 6.78 (q, J = 7.1 Hz, 1H), 7.57 (m, 2 H), 7.67 (m, 1 H), 8.42 (m, 2 H),

*Synthesis of **10***

To a mixture of 1.26 g (11.15 mmol) of N,N-dimethylprenylamine and 3 mL of THF (dried over sodium and distilled under nitrogen) under nitrogen was added 2.73 g (11.15 mmol) of 9-bromo-9H-fluorene. The resulting mixture was stirred for 12 h. The solid thus precipitated out was washed with twice 25 mL portions of hexanes affording 2.50 g (6.91 mmol, 62%) of **10**. The ^{1}H NMR of the solid was analyzed and compared with the previously reported ^{1}H NMR. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.84 (s, 3 H), 1.88 (s, 3 H), 3.27 (s, 6 H), 4.29 (d, J = 7.8 Hz, 2 H), 5.38 (t, J = 7.8 Hz , 1 H), 6.60 (s, 1

H), 7.37 (t, J=7.5 Hz, 2 H), 7.54 (t, J = 7.5 Hz, 7.5 Hz, 2 H), 7.73 (d, J = 7.5 Hz, 2 H), 7.83 (d, J = 7.5 Hz, 2 H).

*Synthesis of **13***

To a mixture of 1.25 g (9.55 mmol) of N,N-dimethylcinnamylamine and 5 mL of acetonitrile (dried over sodium and distilled under nitrogen) under nitrogen was added 2.34 g (9.55 mmol) of 9-bromo-9H-fluorene. The resulting mixture was stirred for 12 h. The solid thus precipitated out was washed with twice 25 mL portions of ether affording 2.90 g (7.73 mmol, 81%) of **13**. The ^{1}H NMR of the solid was analyzed and compared with the previously reported ^{1}H NMR. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.36 (s, 6 H), 4.64 (d, J = 7.5 Hz, 2 H), 6.25 (m, 1 H), 6.54 (s, 1 H), 7.10 (d, J=15.5 Hz, 1 H), 7.34-7.46 (m, 7 H) 7.54 (t, J = 7.5 Hz, 7.5 Hz, 2 H), 7.75 (d, J = 7.5 Hz, 2 H), 7.84 (d, J = 7.5 Hz, 2 H).

*Synthesis of **16***

To a mixture of 1.46 g (6.77 mmol) of 4-Nitrobenzyl bromide and 1 mL of acetonitrile (dried over sodium and distilled under nitrogen) under nitrogen was added 1.09 g (6.75 mmol) of N,N-dimethylcinnamylamine. The resulting mixture was stirred for 30 min for 60 °C. The solid thus precipitated out was washed with twice 25 mL portions of ether affording 1.52 g (4.05 mmol, 60%) of **16**. The ^{1}H NMR of the solid was analyzed and compared with the previously reported ^{1}H NMR. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.28 (s, 6 H), 4.71 (d, J = 8.0 Hz, 2 H), 5.51 (s, 2 H), 6.30 (m, 1 H), 7.07 (d, J = 15.5 Hz, 1 H), 7.31-7.46 (m, 5 H), 8.00 (d, J = 9.0Hz, 2 H), 8.24 (d, J = 9.0Hz, 2 H).

*Synthesis of **19***

To a mixture of 1.00 g (7.62 mmol) of N,N-dimethylalanine methyl ester and 4 mL of hexanes (dried over 4 Å molecular sieves) under nitrogen at room temperature was added 1.14 g (7.65 mmol) of 1-bromo-3-methylbut-2-ene. The resulting mixture was stirred for 16 h. During the stirring some solid precipitated out from the solution. After the solid was dissolved in minimum amount of dichloromethane, approximately 2 mL of THF was added followed by 10 mL of hexanes, and the mixture was again stirred overnight to precipitate out the solid. This precipitation process was repeated twice to afford 1.14 g (4.04 mmol, 53%) of **19**. ^{1}H NMR ($CDCl_3$): δ 1.76 (d, J=7.2 Hz, 3 H), 1.86 (s, 6 H), 3.37 (s, 3 H), 3.44 (s, 3 H), 3.80 (s, 3 H), 4.43 (q, J = 8.1 Hz, 13.5 Hz, 1 H), 4.49 (q, J = 8.06 Hz, 13.48 Hz, 1 H), 4.92 (q, J = 7.2 Hz, 1 H), 5.34 (t, J = 8.1 Hz, 1H). ^{13}C NMR (100.47 MHz, $CDCl_3$): δ 13.6, 19.4, 26.7, 47.5, 48.6, 53.5, 61.7, 67.0, 110.3, 150.0, and 168.8.

Comment: The products obtained by base mediated sigmatropic rearrangement of the ammonium salts have already been reported. The product distribution has been done on the reaction mixture by characterizing the products either from the previously reported ^{1}H NMR data for the [2,3]- and [1,2]- products or by purifying the [2,3]- and [1,2]- products followed by ^{1}H NMR analysis.

*Base-mediated Sigmatropic Rearrangement of **1***

To a mixture of 1.5 mL of acetonitrile (dried over calcium hydride followed by

distilled under nitrogen) and 160 mg (0.51 mmol) of 4 under nitrogen at 25 °C was added 800 mg (5.35 mmol) of DBU dropwise. The mixture was stirred for 12 h at room temperature. Then it was partitioned between 25 mL of ether and 25 mL of water. The ether layer was washed with twice 25-mL portions of water, dried (Na_2SO_4), and the volatiles were removed on a rotatory evaporator to afford 84 mg (72%) of crude **2** (**2** was characterized in the reaction mixture by comparing the ^{1}H NMR of the reaction mixture with the previously reported ^{1}H NMR of **2**) as a mixture of two diastereomers. The product, **2** was purified as a mixture of two inseparable diastereomers by flash chromatography on silica gel using 15% ethyl acetate in hexanes as eluent.

In a closely analogous (identical concentrations) reaction, the outcome of the reaction was studied at 180 °C using DMSO as the solvent. However, **2** was obtained as exclusive product from the reaction.

*Base-mediated Sigmatropic Rearrangement of **4***

To a mixture of 5 mL of acetonitrile (dried over calcium hydride followed by distilled under nitrogen) and 180 mg (0.50 mmol) of **4** under nitrogen at 60 °C was added 56 mg (1 mmol) of pulverized KOH. The mixture was stirred for 15 min at 60 °C. Then mixture was partitioned between 10 mL of ether and 10 mL of water. The ether layer was washed with 20-mL portions of water, dried (Na_2SO_4), and the volatiles were removed on a rotatory evaporator to afford 72 mg (51%) of crude **5** (**5** was identified in the reaction mixture by comparing the ^{1}H NMR of the reaction mixture with the previously reported ^{1}H NMR of **5**).

Base-mediated Sigmatropic Rearrangement of 7

To a mixture of 0.8 mL of acetonitrile (dried over calcium hydride followed by distilled under nitrogen) and 280 mg (0.86 mmol) of **7** under nitrogen at 25 °C was added 650 mg (4.28 mmol) of DBU. The mixture was stirred for 8 h at 25 °C. Then mixture was partitioned between 25 mL of ether and 10 mL of water. The ether layer was washed with two 25-mL portions of water and dried over anhydrous Na_2SO_4. Then the volatiles were removed on a rotatory evaporator to afford 150 mg (61%) crude mixture of **8** and **9**. The ratio of the [2,3]-product **8** and the [1,2]-product **9** was determined to be approximately 3:4 by ^{1}H-NMR analysis. (**8** and **9** was identified in the reaction mixture by comparing the ^{1}H NMR of the reaction mixture with the previously reported ^{1}H NMR of **8** and **9**).

*Base-mediated Sigmatropic Rearrangement of **10***

To a mixture of 10 mL of acetonitrile (dried over calcium hydride followed by distilled under nitrogen) and 1 g (2.8 mmol) of **10** under nitrogen at 25 °C was added 500 mg (3.3 mmol) of DBU. The mixture was stirred for 12 h at 25 °C. Then mixture was partitioned between 25 mL of ether and 10 mL of water. The ether layer was washed with two 25-mL portions of water and dried over anhydrous Na_2SO_4. Then the volatiles were removed on a rotatory evaporator to afford 507 mg (65%) mixture of **11** and **12**. The ratio of the [2,3]-product **11** and the [1,2]-product **12** was determined to be approximately 55:45 by ^{1}H-NMR analysis. The isomers were separated by flash chromatography on silica gel using 10% ethyl acetate in hexanes as eluent. ^{1}H NMR

(500 MHz, $CDCl_3$) **11:** δ 0.95 (s, 6 H), 2.24 (s, 6 H), 5.05 (t, J = 11.0 Hz, J = 6.0 Hz, 2 H), 6.45 (dd, J = 11 Hz, J = 6 Hz, 1 H), 7.24 (m, 2 H) 7.34 (m, 2 H), 7.62 (m, 4 H). ^{1}H NMR (500 MHz, $CDCl_3$) **12**: δ 1.38 (s, 3 H), 1.50 (s, 3 H), 2.21 (s, 6 H), 2.79 (d, J = 7.0 Hz, 2 H), 4.88 (t, J = 7.0 Hz, J = 7.0 Hz, 1 H), 7.26 (t, J = 7.1 Hz , J = 7.7 Hz, 2 H), 7.34 (t, J = 7.1 Hz, J = 7.7 Hz, 2 H), 7.48 (d, J = 7.7 Hz, 2 H), 7.65 (d, J = 7.1 Hz, 2 H). The ^{1}H NMR spectra of **11** and **12** were compared with the previously reported spectra to characterize them unequivocally.

*Base-mediated Sigmatropic Rearrangement of **13***

To a mixture of 10 mL of acetonitrile (dried over calcium hydride followed by distilled under nitrogen) and 2.03 g (5 mmol) of **13** under nitrogen at 25 °C was added 750 mg (5.0 mmol) of DBU. The mixture was stirred for 12 h at 25 °C. Then mixture was partitioned between 50 mL of ether and 10 mL of water. The ether layer was washed with two 25-mL portions of water and dried over anhydrous Na_2SO_4. Then the volatiles were removed on a rotatory evaporator to afford 1.6 g (80%) mixture of **14** and **15**. The ratio of the [2,3]-product **14** and the [1,2]-product **15** was determined to be approximately 82:18 by ^{1}H-NMR analysis. The isomers were separated by flash chromatography on silica gel using 15% ethyl acetate in hexanes as eluent. ^{1}H NMR (500 MHz, $CDCl_3$) **14**: δ 2.34 (s,6 H), 4.41 (d, J=8.5 Hz, 1 H), 5.16 (d, J = 17.2 Hz, 1 H), 5.32 (d, J = 10.5, 1 H), 6.34 (d, J = 7.2 Hz, 2 H), 6.71 (t, J = 7.2 Hz, 2 H), 6.80-6.90 (m, 2 H), 7.21 (m, 2 H), 7.34 (m, 4 H), 7.49 (d, J = 7.5 Hz, 1 H), 7.79 (d, J=7.5 Hz, 1 H).

^{1}H NMR (500 MHz, $CDCl_3$) **15**: δ 2.24 (s, 6 H), 3.00 (d, J = 7.0 Hz, 2 H), 5.85 (td, J = 7.0 Hz, J = 15.9 Hz, 1 H), 6.15 (d, J = 15.9 Hz, 1 H), 7.12 (m, 5 H), 7.30(m, 6 H), 7.52 (d, J=7.4 Hz, 2 H), 7.65 (d, J = 7.1 Hz, 2 H).

The ^{1}H NMR spectra of **14** and **15** were compared with the previously reported spectra to characterize them unequivocally.

*Base-mediated Sigmatropic Rearrangement of **16***

To a mixture of 5 mL of acetonitrile (dried over calcium hydride followed by distilled under nitrogen) and 377 mg (1 mmol) of **16** under nitrogen at 25 °C was added 760 mg (5.0 mmol) of DBU. The mixture was stirred for 16 h at 25 °C. Then mixture was partitioned between 50 mL of ether and 25 mL of water. The ether layer was washed with two 25-mL portions of water and dried over anhydrous Na_2SO_4. Then the volatiles were removed on a rotatory evaporator to afford 216 mg (80%) mixture of **17** and **18**. The ratio of the [2,3]-product **17** and the [1,2]-product **18** was determined to be approximately 3:1 by ^{1}H-NMR analysis. (**17** and **18** was identified in the reaction mixture by comparing the ^{1}H NMR of the reaction mixture with the previously reported ^{1}H NMR of **17** and **18**).

*Base-mediated Sigmatropic Rearrangement of **19***

To a mixture of 1.5 mL of acetonitrile (dried over calcium hydride followed by distillation under nitrogen) and 1.58 g (5.63 mmol) of **19** under nitrogen at 90 °C was added 1.53 g (10.0 mmol) of DBU dropwise. The mixture was stirred for 2 h at 90 °C.

After cooling the reaction mixture to room temperature, it was partitioned between 25 mL of ether and 25 mL of water. The ether layer was washed with five 25-mL portions of water, dried (Na_2SO_4), and the volatiles were removed on a rotatory evaporator to afford 779 mg (3.88 mmol, 69%) of mixture of **20** and **21**. The ratio of the [2,3] product **20** and the [1,2] product **21** was determined to be approximately 80:20 by ^{1}H-NMR analysis. The isomers were separated by flash chromatography on silica gel using 20% ethyl acetate in hexanes as eluent.

20: ^{1}H NMR ($CDCl_3$): δ 1.06 (s, 3 H), 1.14 (s, 3 H), 1.16 (s, 3 H), 2.20 (s, 6 H), 3.70 (s, 3 H), 5.01 (t, J = 6.8 Hz, J= 11.3 2 H), 6.24 (q, J = 6.8 Hz, J= 11.3 2 H, 1 H). ^{13}C NMR ($CDCl_3$): 9.1, 24.5, 25.0, 41.3, 42.7, 51.6, 72.8, 111.8, 145.6 and 175.4. **21**: ^{1}H NMR (C_6D_6) δ 1.34 (s, 3 H), 1.51 (s, 3 H), 1.64 (s, 3 H), 2.29 (s, 6 H), 2.55 (m, 2 H), 3.34 (s, 3 H), 5.38 (t, J = 7.2 Hz, 1 H). ^{13}C NMR (75 MHz, $CDCl_3$): 18.6, 20.4, 26.6, 36.4, 40.2, 51.1 66.6, 120.9, 134.1, 174.4.

Product Ratio versus Temperature

To a mixture of 1.5 mL of acetonitrile (dried over calcium hydride followed by distilled under nitrogen) and 300 mg (1.07 mmol) of **19** under nitrogen at 90 °C was added 305 mg (2.00 mmol) of DBU dropwise. From the reaction mixture 0.30-mL aliquots were withdrawn at 30-min, 60-min and 120-min. The aliquots were diluted with 10 mL of diethyl ether and the mixture was washed with three 5-mL portions of water and dried (Na_2SO_4), and the volatiles were removed on a rotatory evaporator. The ratio of the [2,3] product **20** and the [1,2] product **21** was then evaluated by ^{1}H-NMR analysis.

In closely analogous reactions (identical concentrations), the product ratio was determined at 70 °C, 50 °C, and room temperature. The resulting product ratios, determined by ^{1}H NMR analysis.

In a control experiment, 210 mg of a 95:5 mixture of **20** and **21** was heated at 90 °C for 20 h in 1 mL of acetonitrile in in presence of 0.3 mL of DBU. The proportion of **20** to **21** was unaltered based on NMR analysis.

*Rearrangement of **19** Using Potassium Hydride*

A 50% suspension of potassium hydride in paraffin oil (800 mg, 10 mmol) was rinsed with pentane, and 5 mL dichloromethane was added, followed by the slow addition of 1.00 g (3.57 mmol) of **19**. The reaction mixture was allowed to stir overnight at room temperature then quenched by the slow addition of 1 mL of water at 0 °C. The reaction mixture was partitioned between 25 mL of ether and 25 mL of water, and the ether layer was dried over anhydrous potassium carbonate. The volatiles were removed on a rotary evaporator, and the ratio of **20** and **21** by ^{1}H-NMR analysis was 95:5.

Synthesis of 3-Methyl-2-buten-1,1-d_2-1-ol

To a mixture of 40 mL of diethyl ether (dried over sodium followed by distillation under nitrogen) and 476 mg (11.33 mmol) of $LiAlD_4$ under nitrogen at 0 °C was added dropwise 1.92 g (14.98 mmol) of ethyl 3-methylcrotonate. The mixture was heated to reflux for 1 h then cooled to 0 °C and quenched by the sequential dropwise addition of 0.5 mL of water, 0.5 mL of 15% aqueous sodium hydroxide, and 1.5 mL of

water. The resulting mixture was filtered and filtrate was dried over anhydrous magnesium sulfate. The ether was carefully removed on a rotatory evaporator to afford 957 mg (9.89 mmol, 66%) of crude 3-methyl-2-buten-1,1-d_2-1-ol, contaminated with ether but judged to be approximately 90% pure by NMR analysis. This material was used in the next step without further purification. ^{1}H NMR ($CDCl_3$): δ1.68 (d, J = 1.2 Hz, 3 H), 1.74 (d, J = 1.2 Hz, 3 H), 5.40 (br s, 1 H).

Synthesis of 1-Bromo-3-methyl-2-butene-1,1-d_2

To a mixture of 957 mg (10.8 mmol) of 3-methyl-2-buten-1,1-d_2-1-ol and 15 mL of pentane under nitrogen at 0 °C was added 1.14 g (4.21 mmol) of phosphorus tribromide over a 20-min period. Stirring of the reaction mixture was continued for additional 2 min before addition of 1 mL (24.7 mmol) of ice-cold methanol. To that mixture 10 mL of 5% aqueous ice-cold sodium bicarbonate solution was added followed by washing the organic layer with 5 mL of ice-cold water and 5 mL of ice-cold brine. The pentane layer was dried over anhydrous magnesium sulfate. The solvent was removed on a rotatory evaporator, keeping the temperature at 0 °C, to afford 635 mg of crude 1-bromo-3-methyl-2-butene-1,1-d_2 (6.69 mmol, 62%), judged to be approximately 90% pure by NMR analysis. The crude material was used in the next step without further purification. ^{1}H NMR (399.53 MHz, $CDCl_3$): δ1.73 (d, J = 1.3 Hz, 3 H), 1.78 (d, J = 1.3 Hz, 3 H), 5.52 (br s, 1 H).

Synthetsis of N,N-Bis(methyl-d_3)alanine Methyl Ester

To a mixture of 1.00 g (11.55 mmol) of bis(methyl-d_3)amine hydrogen chloride, 1 mL water and 600 mg (15 mmol) of sodium hydroxide at 0 °C was added a solution of 831 mg (4.98 mmol) of methyl 2-bromopropanoate in 2 mL of dichloromethane. After stirring overnight the reaction mixture was poured into 20 mL of water and extracted with three 25-mL portions of diethyl ether. The ether layers were combined and dried over anhydrous potassium carbonate, and the volatiles were removed on a rotatory evaporator to afford 459 mg (3.39 mmol, 68%) of crude *N*,*N*-bis(methyl-d_3)alanine, methyl ester, which was used in the next step without further purification. ^{1}H NMR ($CDCl_3$): δ 1.27 (d, J = 7.0 Hz, 3 H), 3.22 (q, J =7.0 Hz 1 H), 3.70 (s, 3 H).

*Synthesis of **19-d_8***

To a mixture of 459 mg (3.35 mmol) of *N*,*N*-bis(methyl-d_3)alanine, methyl ester and 2 mL of hexanes under nitrogen at room temperature was added 525 mg (3.48 mmol) of 1-bromo-3-methyl-2-butene-1,1-d_2. The resulting mixture was stirred for 16 h. During the stirring some solid precipitated out from the solution. After the solid was dissolved in minimum amount of dichloromethane, approximately 1 mL of THF was added followed by 5 mL of hexanes. Then mixture was again stirred overnight to precipitate out the solid. This process was repeated twice to afford 596 mg (2.08 mmol, 62%) of the ammonium salt (**19**-d_8). ^{1}H-NMR ($CDCl_3$): δ 1.76 (d, J=7.1 Hz, 3 H), 1.89 (s, 6 H), 3.83 (s, 3 H), 4.92 (q, J = 7.1 Hz, 1 H), 5.01 (br s, 1 H).

*Crossover Rearrangement of **19 / 19-d_8***

To a mixture of 280 mg (1.00 mmol) of **19**, 288 mg (1.00 mmol) of **19**-d_8, and 2.8 mL of acetonitrile (dried over calcium hydride followed by distilled under nitrogen) under nitrogen at 90 °C was added 570 mg (3.74 mmol) of DBU dropwise. The stirring of the reaction mixture continued for additional 1 h at 90 °C. After cooling to room temperature the reaction mixture was partitioned between 25 mL of ether and 25 mL of water. The ether layer was washed with five 25-mL portions of water and dried (Na_2SO_4), and the volatiles were removed on a rotary evaporator. The residue was flash chromatographed on silica gel using 20% ethyl acetate in hexanes as eluent, and the separated components **20** and **21** were characterized by ^{1}H-NMR and ESI-MS. In each case the extent of crossover was based on the relative intensities of the M=206 and M=208 peaks, averaging two measurements for **20** and three measurements for **21**, to obtain 4.9% and 17.9% for **20** and **21**, respectively.

A closely analogous reaction (identical concentrations) was performed at room temperature. The purified **20** was analyzed by ESI-MS. In that case the extent of crossover is negligible.

Synthesis of Methyl-d_3 Bromopropionate

To a mixture of 3.20 g (88.0 mmol) of d_4-methanol, 3.48 g (44.0 mmol) of pyridine and 10 mL of dichloromethane (dried over 3Å molecular sieves) under nitrogen at 0° C was added dropwise slowly 9.50 g (44.0 mmol) of 2-bromopropionyl bromide. The mixture was allowed to stir for 2 h, then quenched by the addition of 50 mL of 15%

aqueous sulfuric acid at 0 °C. The organic layer was washed with two 25-mL portions of water and two 25-mL portions of saturated aqueous sodium bicarbonate solution. After drying over anhydrous magnesium sulfate the volatiles were removed on a rotatory evaporator to afford 6.8 g (39.6 mmol, 90%) of crude methyl-d_3 bromopropionate. ^{1}H NMR ($CDCl_3$): δ 1.84 (d, J = 7.0 Hz, 3 H), 4.38 (q, J = 7.0 Hz, 1 H).

Synthesis of N,N-dimethylalanine Methyl-d_3 ester

A mixture of 4.50 g (39.55 mmol) of 40% aqueous solution of dimethylamine and 4 mL of acetonitrile was cooled to 0 °C in an ice-bath. After cooling, 3.37 g (19.82 mmol) of methyl-d_3 bromopropanoate was added and the mixture was stirred at 0 °C for 12 h. The stirring was continued further for 12 h at room temperature. The reaction mixture was then poured into 20 mL of water and the organics extracted with three 50-mL portions of diethyl ether. The ether extracts were combined and dried over anhydrous sodium sulfate. The ether was then removed on a rotatory evaporator to afford 1.00 g (7.53 mmol, 38%) crude N,N-dimethylalanine methyl-d_3 ester, judged to be more than 95% pure by NMR analysis. ^{1}H NMR $CDCl_3$: δ 1.29 (d, J = 7.4 Hz, 3 H), 2.34 (s, 6 H), 3.24 (q, J =7.4 Hz 1 H).

*Synthesis of **19-d_5***

To a mixture of 500 mg (3.72 mmol) of N,N-dimethylalanine methyl-d_3 ester and 2 mL of hexanes under nitrogen at room temperature was added 559 mg (3.70 mmol) of 1-bromo-3-methyl-2-butene-1,1-d_2. The resulting mixture was stirred for 16 h.

During the stirring some solid precipitated out from the solution. After the solid was dissolved in minimum amount of dichloromethane, approximately 1 mL of THF was added followed by 5 mL of hexanes. Then mixture was again stirred overnight to precipitate out the solid. This process was repeated twice to afford 709 mg (2.48 mmol, 67%) of the ammonium salt (**19**-d_5).

*Crossover Rearrangement of **19 / 19-d_5***

To a mixture of 185 mg (0.66 mmol) of **19**, 190 mg (0.67 mmol) of **19**-d_5, and 1.8 mL of acetonitrile (dried over calcium hydride followed by distilled under nitrogen) under nitrogen at 90 °C was added 370 mg (2.43 mmol) of DBU dropwise. The stirring of the reaction mixture continued for additional 1 h at 90 °C. After cooling to room temperature the reaction mixture was partitioned between 25 mL of ether and 25 mL of water. The ether layer was washed with five 25-mL portions of water and dried (Na_2SO_4), and the volatiles were removed on a rotary evaporator. The residue was flash chromatographed on silica gel using 20% ethyl acetate in hexanes as eluent, and the separated components **20** and **21** were characterized by ^{1}H-NMR and ESI-MS. In each case the extent of crossover was based on the relative intensities of the M=203 and M=205 peaks. The extent of crossover in **20** was found to be 9% while in **21** the extent was 26%.

CHAPTER V

MECHANISTIC INVESTIGATION AND METHODOLOGY DESIGNING OF SOMMELET-HAUSER REARRANGEMENT AND STEVENS REARRANGEMENT

Our study, discussed in the previous two chapters, suggests that the competition between formally allowed [2,3]-sigmatropic rearrangements and forbidden [1,2]-sigmatropic rearrangements is a result of partitioning of dynamic trajectories passing through a single, [2,3]-rearrangement TS. The study suggested that aromatic [2,3]-rearrangement TS promote the cleavage path leading to diradicals. Those diradicals then can recombine to give both [2,3]- and [1,2]-products.

That study dealt with rearrangement associated with allylic systems. However, the oldest and most frequent cases of competition have been observed with benzylic systems. In principle, the role of the benzylic and allylic part of ylides should be the same. But in the benzylic systems the concerted [2,3]-rearrangement TS requires at least partial disruption of aromaticity of the phenyl ring. This triggered a very important mechanistic question. There are two possibilities. First, it is possible that the [2,3]-TS involving the phenyl ring still has considerable pericyclic stabilization and thus the competition arises due to partitioning of dynamic trajectories. It may also be possible that due to disruption of aromaticity of the phenyl ring the [2,3]-rearrangement becomes less favorable and the competition of [2,3]- and [1,2]-rearrangement arises due to small energy difference between the pericyclic [2,3]-rearrangement and cleavage TS. This

mechanistic question intrigued us and we decided to study the competition between traditional Sommelet-Hauser and Stevens rearrangements by a combination of experiments and theoretical calculations.

Mechanistic understanding of reactions has laid the foundation for synthetic methodology development. However, synthetic methodology development commonly relies on a qualitative understanding of reaction mechanisms. This qualitative understanding is necessary but often not sufficient to control synthetic outcomes. This is because theoretical modeling of a reaction systems requires consideration of many factors. As a result, rigorous theoretical calculations are often necessary for sufficiently accurate modeling. We envisioned that rational synthetic methodology development required a deep understanding of the reaction system involved. For this reason, we sought to develop our methodology based on the results of the theoretical calculations. In this chapter, besides a mechanistic study we describe a rational methodology development via theoretical calculations to control the [2,3]- and [1,2]-product distribution.

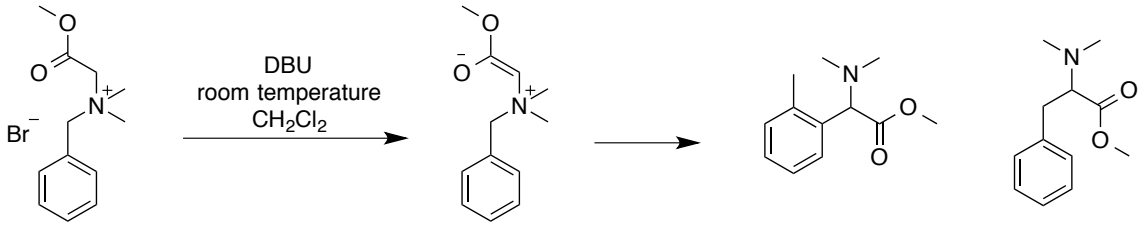
Experimental Results and Discussions

Firstly, we sought a detailed study to understand the mechanism of sigmatropic rearrangements of benzyl ammonium ylides. Primarily, this would test whether our hypothesis held regarding the competition between [2,3]- and [1,2]-rearrangement on benzylic systems. Secondly, we envisioned that the understanding of the mechanism

could be utilized to control the selectivity when there is a competition between [2,3]- and [1,2]-rearrangements.

We decided to study a benzylic system, which is structurally similar to the allylic systems which we previously studied (CHAPTER III and IV). We first decided to study base mediated sigmatropic rearrangement of the ammonium salt **1**. When the ammonium salt, **1** was treated with DBU at 25 °C in dichloromethane a mixture of [2,3]-product (**2**) and [1,2]- product (**3**) was obtained (Scheme 5-1). The ratio of **2** to **3** was found to be 55:45 by ^{1}H-NMR analysis.

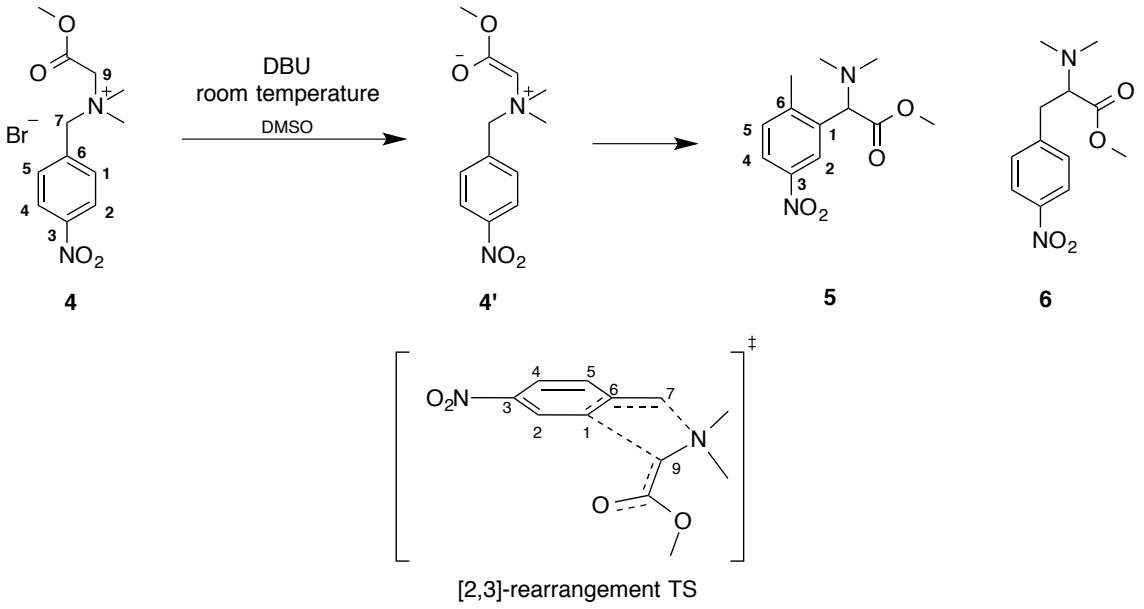
Scheme 5-1



As KIEs provide important structural information about the TS we decided to measure KIEs on the [2,3]-product, **2** to acquire information about the TS geometry of the [2,3]-sigmatropic rearrangement. However, ^{13}C-NMR spectra of **2** revealed that the peaks of interest were very close to other peaks. For this reason it was not possible to measure KIEs on the [2,3]-product **2** by Singleton's NMR methodology.[32] After facing

this difficulty we decided to measure KIEs on another system, which was structurally similar to **1.** We found that a new compound **4** (4-nitro substituted) on treatment with DBU in DMSO at room temperature gives a mixture of **5** ([2,3]-product) and **6** ([1,2]-product) (Scheme 5-2). The ratio of **5** to **6** was found to be 34:66 by ^{1}H-NMR analysis. In this case, the peaks of interest in ^{13}C-NMR spectra of **5** were well separated. Hence those peaks could be integrated to measure KIEs.

Scheme 5-2



Measurement of intermolecular KIEs on **5** was not possible due to difficulties in converting **4** to **5** quantitatively. However, measurement of intramolecular KIEs was

possible on **5**. In **4**, C^1 and C^5 are equivalent. However during the [2,3]-rearrangement only one of them participates in the rearrangement process and ends up as C^1 in the product, **5** (Scheme 5-2). To measure intramolecular KIE a homogenous mixture of DMSO and **4** was treated with DBU at room temperature. Then from the reaction mixture **5** was recovered and the relative ^{13}C abundance in C^5 to C^1 was measured by NMR methodology to determine intramolecular KIE. A closely analogous reaction was carried out for duplicate measurement of KIE. The experimental KIE is summarized in Table 5-1.

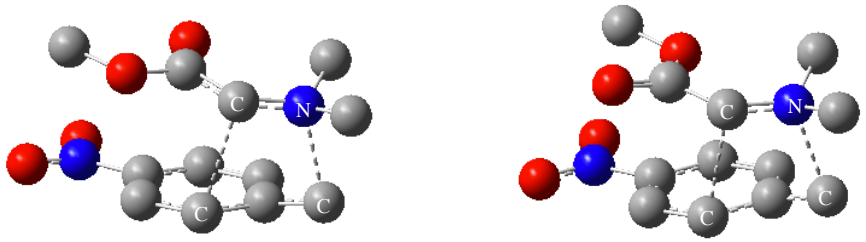
Table 5-1. Experimental intramolecular KIEs for rearrangement of **4** to **5**

Experiment	Relative amount of ^{13}C (C^1/C^5) in **5**	Intramolecular KIE (C^1/C^5) in **5**
1	0.984	1.005(0.002)
2	0.986	1.003(0.002)

Very small intramolecular KIE suggests that at the TS the interaction between the carbons (C^1 and C^9) eventually form the bond is very weak. This structural feature of the TS is similar to the TS of the allylic system (compare Table 3-2 with Table 5-1). After that we sought to predict the experimental KIEs in order to theoretically probe the reaction.

Theoretical Study and Discussions

In order to predict KIEs, we located two low energy TSs for the [2,3]-rearrangement of **4′, TS1** and **TS2** (Figure 5-1).



TS1(0.0 kcal/mol) **TS2(2.6 kcal/mol)**

Figure 5-1. Two lowest energy TSs of [2,3]-rearrangement of **4′**(H-atoms were deleted for clarity)

The predicted KIEs differ considerably depending upon the method used. However, one key feature about all the predicted KIEs was that the KIEs were small indicating very weak interaction between the carbon centers that would form the bond. This can be justified by the fact that at the TS the predicted C^1-C^9 distances are quite large compared to C^7-N distances (Table 5-2).

Table 5-2. KIE predictions (25 °C, k_{12C}/k_{13C}) versus C^7-N andC^1-C^9 distances

Entry	Method	KIE	C^7-N distance	C^1-C^9 distance
Experimental	-	1.005(2) 1.003(2)		
1	B972	1.002	2.136	3.042
2	M062X	1.005	2.186	2.746
3	APFD	1.003	2.052	2.864
4	B3LYP	1.002	2.103	3.111
5	BP86	1.001	1.991	3.303
6	B98	1.002	2.145	3.038
7	lc-B97D	1.006	2.195	2.728
8	MN12L	1.005	2.019	2.957
9	MN12SX	1.002	2.074	2.928
10	N12SX	1.002	2.151	2.917
11	PBE0D3	1.003	1.947	3.176
12	PBE0	1.003	2.089	2.831
13	B3LYPD2	1.001	2.009	2.990
14	B97D	1.000	1.876	3.072
15	M11	1.005	2.251	2.664
16	N12	1.001	2.003	3.141
17	PBE	1.001	1.985	3.150
18	SOGGA11X	1.003	2.197	2.865
19	WB97XD	1.004	2.195	2.772
20	WB97X	1.005	2.230	2.727
21	WB97	1.005	2.229	2.697
22	PBED2	1.001	1.928	2.979

Table 5-2. Continued

Entry	Method	KIEs	C^7-N distance	C^1-C^9 distance
23	BP86D2	1.001	1.899	2.958
24	BLYPD2	1.000	1.869	3.081
25	B3LYPD3	1.001	2.010	2.963
26	M11L	1.003	1.978	2.986
27	B97D3	1.000	1.876	3.072
28	B971	1.002	2.135	3.023

[a]Calculations were done with 6-31+G**/PCM(DMSO)

We inferred that the theoretically located TS, **TS1** for the benzylic system showed similar structural features to that of the allylic system. Encouraged by this result we sought to investigate the competition between [2,3]- and [1,2]-rearrangement of **4′**.

Since the ylide (**4′**) is a charge separated species we sought to examine possible interactions of the ylides with the protonated base. To test the involvement of protonated DBU during the rearrangement, the reaction was carried out with potassium hydride (KH) as base in DMSO in the presence of 18-Crown-6. The KH-mediated rearrangement afforded exclusively the [1,2]-product (**6**). This suggested two possibilities. Firstly, presence of DBU favors the formation of the [2,3]-product (**5**). The other possibility was that the [2,3]-product (**5**) formed but decomposed in the reaction mixture. The possibility of decomposition was ruled out when treatment of the [2,3]-product (**5**) with KH/18-Crown-6 in DMSO did not lead to any decomposition. This indicated that DBU

somehow favors formation of **5**. We have addressed this mechanistic question in a later part of this chapter.

We should expect that when KH was used in there was species in the reacyion mixture that could interact with the ylide. This means in the absence of such interactions, **4′** rearranges exclusively to **6**. First we wanted to utilize TST to account for the experimental outcome.

For this purpose we needed the free energy difference between the [2,3]-rearrangment TS (**TS1**) and the cleavage-TS (**TS′1**), Figure 5-1 and Figure 5-2.

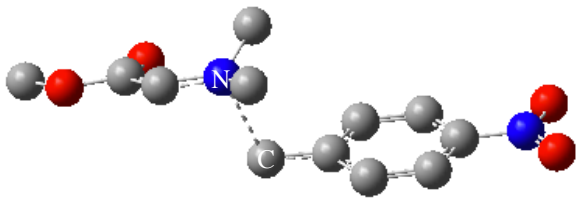


Figure 5-2. TS of C-N bond cleavage of **4′** (H-atoms have been omitted for clarity)

After locating the cleavage TS we calculated, the free energy difference between the [2,3]-rearrangement TS (**TS1**) and the cleavage TS (**TS′1**). The difference between the free energies of the TSs is summarized in Table 5-3. Irrespective of the method used

it was found that the [2,3]-rearrangement TS was of lower energy compared to the cleavage TS. Hence TST failed to account for the experimental outcome.

Table 5-3. Prediction of concerted versus cleavage path based on TST

Method[a]	**[2,3]-rearrangment TS**[b]	**Cleavage TS**[b]	**Energy difference**[c]	**Ratio of [2,3]- to cleavage**
B3LYPD2	-877.032875	877.035656	1.75	19.2:1
B3LYP	-876.985233	876.985471	0.15	1.3:1
M062X	-876.584549	876.591218	4.18	1194.3:1

[a]6-31+G**/PCM(DMSO).[b]Energy in Hartree/Particle. [c]Energy in kcal/mol

Since TST failed to account for the experimental results we envisioned that dynamic effects might be responsible for the experimental outcomes.

Since the KIE predicted by M062X was in fairly good agreement with experimental results, we employed the TS located by that method to run dynamic trajectories. It is important to note that we decided to run trajectories on the [2,3]-TS located using a smaller basis-set (6-31G*) because of limited computational power. The outcomes of the dynamic trajectory calculations are summarized in Table 5-4.

Table 5-4. Outcome of trajectories passing through **TS1**

Method/Basis Set/Solvent Model	Rearrangement:Cleavage
UM062X/6-31G*/PCM[a,b]	2:15 (12%:88%)
Experimental[b]	Exclusive cleavage

[a]Quasiclassical, [b]25 °C.

From Table 5-4, it quite evident that most of the trajectories from the [2,3]-TS ended up as the diradicals and only a small portion of the trajectories ended up as the [2,3]-product. However, experimentally when KH was used as the base **4** exclusively ended up to **6** indicating exclusive diradicals formation from **4′**. This means dynamic trajectories from the [2,3]-TS predicted lesser extent of cleavage compared to the experimentally observed extent of cleavage. This could be explained the following way. We saw in Table 4-4 that when we used the TS from M062X for running dynamic trajectories we ended up predicting lesser extent of cleavage compared to the extent observed experimentally. So we suggest that a similar systematic error might be associated with the benzylic system under study.

Considering the results from dynamic trajectory calculations, we propose here that the competition between the [2,3]- and [1,2]-rearrangement in **4** resulted from dynamic partitioning of trajectories passing through **TS1**.

Mechanistic Study Regarding Effect of H-bonding

Even though we were able to explain the origin of experimental results of rearrangement of **4′** we have not answered a very fundamental mechanistic question. Why does DBU favor the concerted (rearrangement) path? In the next section we discuss the mechanistic investigation that unraveled the origin of that experimental observation.

Experimentally, we found that when **4** was treated with DBU in DMSO the ratio of **5** to **6** was 33:67 while with KH **6** was found to be the exclusive product. There might be different reasons of this experimental observation. However, we hypothesized that the origin of this outcome was due to hydrogen bonding (H-bonding) between the protonated DBU and the carbonyl oxygen of **4′** at the TS. In order to investigate our hypothesis we sought to explore the effect of H-bonding. This was achieved by using protic solvents. However, if DBU is used as the base to generate the ylide, protonated DBU will be present in the reaction medium and might be involved in the H-bonding. In order to eliminate this possibility, we decided to use a strong anionic base. We used NaOMe as the base and DMSO (dielectric constant, $\varepsilon = 46.7$), methanol ($\varepsilon = 32.7$) and dichloromethane ($\varepsilon = 8.93$) as the solvents at 25 °C. Among the mentioned solvents, only methanol is a protic solvent. It is important to note that we decided not to use KH or NaH as the base because these bases deprotonate methanol to generate the methoxide. We reacted **4** with NaOMe in the mentioned solvents and measured the product distribution. The experimental product distributions are summarized in Table 5-5.

Table 5-5. Product distribution of NaOMe mediated rearrangement of **4**.

Solvent	Dielectric constant(ε)[a]	% of **5**	% of **6**
DMSO	46.7	-	100
DCM	8.9	-	100
MeOH	32.7	75	25

[a]We chose to use dielectric constant as the parameter of polarity because it has physical significance.

Table 5-5 clearly indicates that a protic solvent favors the formation of **5** and solvent polarity had no effect on the product distribution. Since experimental results suggested that H-bonding had an effect on product distribution we sought to understand the effect of hydrogen bonding at the TS using theoretical calculations. We located a [2,3]-TS (**TSM1**) with a methanol molecule interacting with the carbonyl oxygen via H-bonding (Figure 5-3). We also located the cleavage TS with a methanol molecule (**TSM′1**) (Figure 5-3).

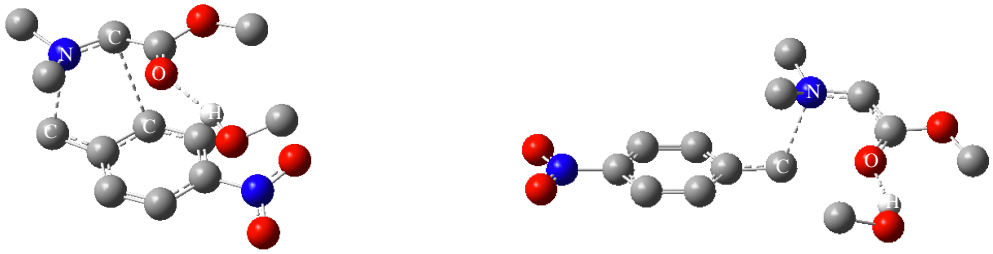


Figure 5-3. [2,3]-rearrangement and C-N cleavage TS with a methanol molecule. Only the H-atom involved in H-bonding was not deleted

Calculations based on TST indicated that the presence of methanol molecule would favor the cleavage path (Table 5-6). Hence, we inferred that TST failed to account for the experimental observation.

Table 5-6. Prediction of product ratio of rearrangement of **4′** based on TST

Method	Energy of [2,3]-TS	Energy of cleavage TS	Free energy difference between the TS
M062X[a]	-876.584549[b]	876.591218 [b]	4.18 [c]
M062X[a]	-992.232493 [b]	-992.22675 [b]	3.60 [c]

[a]6-31+G**/PCM(DMSO), [b]Hartree/Particle, [c]kcal/mol and positive value indicates [2,3]-rearrangment TS of lower energy.

As TST failed to account for the experimental results, we sought a detailed examination of the effect of the methanol molecule on TSs. When there was no

interacting methanol molecule, C^7-N distance in **TS′1** was 2.27 Å while in **TSM′1** the distance changed to 2.28 Å. The difference was very small suggesting a nominal effect of the methanol molecule on the cleavage TS. After that, we examined the effect of an interacting methanol molecule on the [2,3]-rearrangement TS. We found that in **TS1,** C^7-N and C^1-C^9 distances were 2.18 Å and 2.74 Å respectively while in **TSM1** they were 2.36 Å and 2.65 Å. Clearly, the effect of the methanol molecule on the [2,3]-rearrangement TS was significant. Since an interacting methanol molecule decreases the C^1-C^9 distance at the TS it is reasonable to assume that the presence of a methanol molecule increases the interaction between the carbons (C^1 and C^9) that are going to form the bond in the [2,3]-rearrangement. We hypothesized that this increased interaction between C^1 and C^9 tilts the dynamic partitioning towards the concerted path.

To examine our hypothesis, we carried out dynamic trajectory calculations on **TSM1**. The outcome of the dynamic trajectories has been summarized in Table 5-7.

Table 5-7. Outcome of trajectories passing through **TSM1**

Method/Basis-set/Solvent Model	**Rearrangement:Cleavage**
UM062X/6-31G*/PCM(DMSO)[a,b]	45:4 (91% : 9%)
Experimental[b]	75% : 25%[c]

[a]Quasiclassical, [b]25 °C, [c][2,3]- to [1,2]-product ratio when equivolume mixture of DMSO and methanol was used.

From Table 5-7 it is quite clear that the interaction of a methanol molecule via hydrogen bonding tilted the partitioning of the dynamic trajectories towards concerted rearrangement. In other words, dynamic trajectory calculations predicted that the presence of a methanol molecule would favor the [2,3]-rearrangement. This prediction is in agreement with the experimental observations.

Methodology Development

As results from experiments and theoretical calculations suggested that H-bonding favors the concerted path over the cleavage path we envisioned that we could utilize this effect to control the product distribution in rearrangement of benzylic ammonium ylides.

We sought to increase the extent of the concerted path by amplifying the strength of the H-bonding. We hypothesized that as the polarity of the solvent decreased the interactions between the charged and charge separated species in the reaction medium would increase. That means the strength of the H-bonding between the protonated base and ylide should increase as we decrease the polarity of the solvent. Based on our hypothesis we studied the DBU mediated rearrangement of **4** in solvents of different polarities. The experimental results of our study are summarized in Table 5-8.

Table 5-8. Base-mediated rearrangement of **4** in different solvents

Entry	Solvent	Base	ε	Temperature	% of 5	% of 6
1	CCl_4	DBU	2.2	25 °C	99	1
2	Dichloromethane	DBU	8.9	25 °C	94	6
3	2-Butanone	DBU	18.5	25 °C	89	11
4	Acetone	DBU	20.7	25 °C	80	20
5	Ethanol	DBU	24.5	25 °C	89	11
6	Methanol	DBU	32.7	25 °C	75	25
7	DMF	DBU	36.7	25 °C	47	53
8	Acetonitrile	DBU	37.5	25 °C	45	55
9	DMSO	DBU	46.7	25 °C	33	67
10	DMSO	KH	46.7	25 °C	0	100
11	Dichloromethane	KH	8.9	25 °C	0	100

It is important to note that for aprotic solvents, the extent of formation of the [2,3]-product increased with decrease in polarity. Moreover, ethanol, a protic solvent afforded more [2,3]- product compared to acetone, even though the latter was less polar. These results were in agreement with our hypothesis. Interestingly, Table 5-8 showed that we completely switched the product selectivity of the base induced rearrangement by affecting the strength of the hydrogen bond (Entry 2 and 10).

Based on our hypothesis about the effect of hydrogen bonding we expected similar observations on base-mediated rearrangement of **1**.When we treated **1** with KH in dichloromethane, **1** exclusively afforded **3**. This result not only supported our

hypothesis but also expanded the scope of the proposed methodology development.

Conclusion

In CHAPTER III and IV we studied base mediated rearrangment of allyl ammonium ylides. Our mechanistic investigation in CHAPTER III and IV suggested that the competition of allowed [2,3]- and forbidden [1,2]-rearrangment results from the partitioning of dynamic trajectories from the formal [2,3]-rearrangement TS. However, we decided to examine the validity of our hypothesis in other systems.

Literature reports suggested that the competition in benzyl ammonium ylides is more prevalent compared to allyl systems. It could be suggested that the [2,3]-rearrangement TS in case of benzylic system is particularly disfavored due to the disruption of aromaticity of the phenyl ring. Encouraged by our study based on allyl ammonium systems we sought to investigate rearrangement of benzyl ammonium ylides. Based on our study, we would like to propose that even in the case of the benzylic system, **4′**, the competition between the [2,3]- and [1,2]-rearrangement might result from the partitioning of dynamic trajectories from the formal [2,3]-TS and not due to the energy difference between the [2,3]-rearrangement TS and the cleavage TS.

Even though physical organic chemistry has been highly successful in elucidating the synthetic outcomes of many reactions, it has rarely been used to design synthetic methodology development. However, we utilized our mechanistic understanding and dynamic trajectory calculations to design synthetic methodology. Based on our theoretical designing we not only increased the selectivity of a

rearrangement of benzyl ammonium ylides but also switched the product selectivity. Certainly, our theoretical methodology development has not dislodged conventional synthetic methodology development. However, we believe that our work manifested the potential of theoretical designing to achieve synthetic goal.

Experimental Procedures

General Comment

All chemicals were used without purification unless it was mentioned.

*Synthesis of **1***

To a mixture of 8.55 g (50 mmol) of benzyl bromide in 25 mL of diethyl ether (dried over sodium followed by distilled under nitrogen) under nitrogen at room temperature was added 5.90 g (50 mmol) of N,N-dimethylglycine methyl ester. The resulting mixture was stirred for 24 h. During the stirring solid precipitated out from the solution. The solid was then washed two 10 mL portions of diethyl ether to afford 12.2 g (42.5 mmol, 85%) of **1**. ^{1}H NMR ($CDCl_3$): δ 3.55 (s, 6 H), 3.76 (s, 3H), 5.11 (s, 2 H), 5.31 (s, 2 H), 7.46(m, 3 H), 7.64 (m, 2 H). ^{13}C NMR ($CDCl_3$): 49.3, 52.6, 59.9, 67.0, 126.4, 128.7, 130.4, 132.7, 164.8.

*DBU-mediated rearrangement of **1***

To a mixture of 6.00 g (20.8 mmol) of **1** and 30 mL of DCM (dried over 4 Å

molecular sieves) under nitrogen at room temperature was added 6.08 g (40.0 mmol) of DBU. The reaction was stirred for 2.5 h. Then the reaction was partitioned between 25 mL of ether and 25 mL of water. The ether layer was washed with three 25-mL portions of water, dried over dry K_2CO_3, and the volatiles were removed on a rotatory evaporator to afford 509 g (2.5 mmol, 12%) of mixture of **2** and **3**. The ratio of the [2,3] product **2** and the [1,2] product **3** was determined to be approximately 6:4 by ^{1}H-NMR analysis. The isomers have been separated by column chromatography on silica gel using 50% ethyl acetate in hexanes as eluent.

2: ^{1}H NMR ($CDCl_3$): δ 2.26 (s, 6 H), δ 2.42 (s, 3H), 3.65 (s, 3 H), 4.17 (s, 1 H), 7.17 (m, 3 H), 7.51 (m, 1 H). ^{13}C NMR ($CDCl_3$): 19.8, 43.2, 51.9, 70.36, 126.3, 127.9, 128.2, 130.6, 135.0, 137.0, and 172.4.

3: ^{1}H NMR ($CDCl_3$): δ 2.39 (s, 6H), 2.94 (dd, J=13.8 Hz, J=5.9 Hz, 1 H), 3.05 (dd, J=13.8 Hz, J=9.0 Hz, 1 H), 3.43 (dd, J=5.9 Hz, J=9.0 Hz, 1 H), 3.59 (s, 3 H), 7.19 (m, 3 H), 7.27 (m, 2H) ^{13}C NMR ($CDCl_3$): 35.8, 41.9, 51.0, 69.6, 126.4, 128.4, 129.1, 138.2 and 171.9.

*Synthesis of **4***

To a mixture of 12.95 g (60 mmol) of 4-nitrobenzyl bromide and 50 mL of dichloromethane (dried over 4 Å molecular sieves) under nitrogen at room temperature was added 7.02 g (60 mmol) of N,N-dimethylglycine methyl ester. The resulting mixture was stirred for 12 h. During the stirring solid precipitated out from the solution. The liquid phase was decanted off. The solid was then washed two 10 mL portions of

dichloromethane to afford 15.92 g (47.4 mmol, 79%) of **4**. ^{1}H NMR (CDCl3): δ 3.60 (s, 6 H), 3.83 (s, 3H), 5.13 (s, 2 H), 5.61 (s, 2 H), 8.00 (d, J=8.6 Hz, 2 H), 8.34 (d, J=8.6 Hz, 2 H).

*DBU-mediated Rearrangement of **4** and Sample Preparation for Kinetic Isotope Effects*

To a mixture of 10.00 g (30.13 mmol) of **4** and 40 mL of DMSO (dried over 4 Å molecular sieves) under nitrogen at room temperature was added 1.63 g (10.7 mmol) of DBU. The reaction was stirred for 3 h. Then the reaction was partitioned between 50 mL of ether and 25 mL of water. The ether layer was washed with three 25-mL portions of water, dried (K_2CO_3), and the volatiles were removed on a rotatory evaporator to afford 1.98 g (26%) of mixture of **5** and **6**. The ratio of the [2,3] product **5** and the [1,2] product **6** was determined to be approximately 4:9 by ^{1}H-NMR analysis. The isomers have been separated by column chromatography on silica gel using 30% ethyl acetate in hexanes as eluent. The isolated yield of **5** is 470 mg (1.84 mmol, 6.1%) and of **6** is 210 mg (0.63 mmol, 2.7%).

5: ^{1}H NMR ($CDCl_3$): δ 2.30 (s, 6 H), 2.52 (s, 3H), 3.72 (s, 3 H), 4.24 (s, 1 H), 7.33 (d, J=9.9 Hz, 1 H), 8.05 (dd, J=9.9 Hz, J=2.64 Hz, 1 H), 8.43 (d, J=2.64 Hz, 1H). ^{13}C NMR ($CDCl_3$): 19.4, 42.6, 51.7, 69.6, 122.3, 123.0, 131.2, 136.9, 144.8, 146.4, and 170.8.

6: ^{1}H NMR ($CDCl_3$): δ 2.37 (s, 6H), 3.01 (dd, J=12.5 Hz, J=6.5 Hz, 1 H), 3.13 (dd, J=12.5 Hz, J=8.2 Hz, 1 H), 3.44 (dd, J=6.5 Hz, J=8.2 Hz, 1 H), 3.64 (s, 3 H), 7.36 (d, J=9.1 Hz, 2 H), 9.15 (d, J=9.1 Hz, 2 H). ^{13}C NMR ($CDCl_3$): 35.3, 41.7, 51.3, 68.7,

123.6, 130.0, 146.3, 146.7 and 171.2.

*General Procedure for Determination of Product Ratio of Base-mediated Rearrangement of **1** and **4**.*

To a mixture of 1 mL of the solvent and 0.5 mmol of the ammonium salt, 0.5 mmol of the base was added at room temperature. The reaction was stirred for 1 h. Then the reaction was quenched with 10 drops of water (extreme care was taken when KH was used as base). Then the mixture was partitioned between 5 mL ether and 5mL water. The ether layer was then washed with two 5-mL portions of water and dried with anhydrous potassium carbonate. Then volatiles were removed on a rotatory evaporator. The product ratio was then determined by ^{1}H-NMR.

CHAPTER VI

CONCLUSION

First, we investigated the mechanism of [2,3]- and [1,2]-sigmatropic rearrangements of allyl N-ylides by a combination of kinetic isotope effects (KIEs), temperature dependence of product distribution, crossover experiments and theoretical calculations. Theoretical calculations suggested "loose" TSs for [2,3]-rearrangements. Our experimental KIEs for [2,3]-rearrangement matched with theoretically predicted KIEs. Our dynamic trajectory calculations revealed that from the "loose" [2,3]-rearrangement TS there is a bifurcation on the free energy surface. One of the paths was concerted that led to the [2,3]-product while other path led to diradicals. Those diradicals then can recombine to give both the [1,2]- and [2,3]-products. In addition, our crossover experiments confirmed the formation of [2,3]-products via a stepwise process. Even though the stepwise path, involving cleavage is enthalpically disfavored, compared to the concerted path, it has an entropic advantage. This entropic advantage of the stepwise path was supported by the observation that higher temperatures favored [1,2]-products. Since there is no bifurcation on the potential energy surface that can lead to the diradicals, we called this dynamic effect entropic bifurcation. Overall we propose here that the common cooccurence of [2,3]- and [1,2]-rearrangement is due to the fact that both are associated with the same TS. We further extended our study to the rearrangements of the benzylic N-ylides. Our mechanistic study revealed that the origin of competition between the [2,3]- and [1,2]- rearrangements is the same as in the cases

of the allyl N-ylides.

Our mechanistic findings suggested that controlling of atomic motions is necessary to achieve selectivity in this competition. This is because this competition arises due to a dynamic effect. Considering this opportunity, we subsequently developed a synthetic methodology via theoretical calculations. We were able to control the selectivity by controlling the atomic motions through hydrogen bonding. Overall the work discussed in this dissertation not only answered a very fundamental mechanistic question but also utilized the mechanistic understandings for synthetic methodology development.

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APPENDIX

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Structures for the Rearrangement of Glycineallylammonium Bromide

Cation-B3LYP-D2/6-31+G/PCM- Conf2**

/home/bibaswanbiswas/c8/23parentSM2B3D2PS

parent sm conf 2

B3LYP/6-31+G**

E(RB3LYP) = -519.576987851

Zero-point correction= 0.240438 (Hartree/Particle)

Thermal correction to Energy= 0.253183

Thermal correction to Enthalpy= 0.254128

Thermal correction to Gibbs Free Energy= 0.201260

Sum of electronic and ZPE= -519.336549

Sum of electronic and thermal Energies= -519.323804

Sum of electronic and thermal Enthalpies= -519.322860

Sum of electronic and thermal Free Energies= -519.375728

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.875	46.943	111.270

C,0,2.0118341603,-0.7967810691,-2.241639745

O,0,2.7688990345,0.4347315652,-2.4047463337

C,0,2.7842096205,0.9649270844,-3.623761134

O,0,2.2179839729,0.507229846,-4.5973435544

C,0,3.6294435895,2.2320931766,-3.5835941847

N,0,3.7213850288,2.9921952502,-4.8798104341

C,0,4.4357083946,2.179678611,-5.9306496582

C,0,4.530204375,4.2344162768,-4.6023149496

C,0,2.3411244626,3.4037716527,-5.4314834853

C,0,1.4724256821,4.0714262579,-4.4099085947

C,0,1.1908370164,5.376710319,-4.4452866791

H,0,2.1314987601,-1.064871835,-1.1931442059

H,0,0.9627734765,-0.6145700232,-2.4853120576

H,0,2.423854689,-1.5680492904,-2.8961962755

H,0,4.6482799399,1.9686235028,-3.289840571

H,0,3.2241543707,2.9079267871,-2.8280874685

H,0,3.8509578196,1.2848221256,-6.1326261033

H,0,4.5211255789,2.7957159768,-6.8264746725

H,0,5.4250562258,1.9254852247,-5.5480441456

H,0,5.5041312858,3.9309010763,-4.2174410393

H,0,4.6421611392,4.7778063685,-5.5404062559

H,0,3.9945626682,4.8402084404,-3.8721706699

H,0,2.5626219619,4.0691680792,-6.2680136907

H,0,1.8905905845,2.4830855693,-5.8007027733

H,0,1.0288377989,3.4380463022,-3.6450556813

H,0,1.6085075895,6.0240991344,-5.213362045

H,0,0.5258627739,5.8285215903,-3.7149065922

23TS-B3LYP-D2/6-31+G/PCM**

/home/bibaswanbiswas/c8/23parentTSB3D2PS

parent ts exo s-cis

B3LYP/6-31+G**

E(RB3LYP) = -519.067923267

Zero-point correction= 0.222213 (Hartree/Particle)

Thermal correction to Energy= 0.234910

Thermal correction to Enthalpy= 0.235854

Thermal correction to Gibbs Free Energy= 0.184094

Sum of electronic and ZPE= -518.845711

Sum of electronic and thermal Energies= -518.833013

Sum of electronic and thermal Enthalpies= -518.832069

Sum of electronic and thermal Free Energies= -518.883829

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.408	47.022	108.938

C,0,1.9918091767,-0.809209825,-2.3262079805

O,0,2.725447739,0.419122139,-2.4545316512

C,0,2.8225841576,0.9292027439,-3.7284625127

C,0,3.481175396,2.1933223282,-3.7204134657

N,0,3.8311322247,2.8820187818,-4.864109122

C,0,4.6775828194,4.0572988169,-4.5778370444

O,0,2.354328585,0.3184629103,-4.7021199114

C,0,4.3223591519,2.1288628785,-6.0383123247

C,0,2.0976924831,3.8277104129,-5.7033721897

C,0,1.5097695154,4.2429428785,-4.4957034072

C,0,0.9963178156,3.312392053,-3.627683994

H,0,2.0137716856,-1.0524431442,-1.2624900804

H,0,0.9590383656,-0.6796055152,-2.6658170947

H,0,2.4641252859,-1.6064361108,-2.9089019046

H,0,3.7212115367,2.6526578882,-2.7730789992

H,0,5.3232805008,1.7345376947,-5.8233166193

H,0,3.6372009994,1.3116380315,-6.2519137224

H,0,4.3707213925,2.8165913473,-6.8857002618

H,0,5.6514695998,3.7284567406,-4.195295962

H,0,4.8134577094,4.6279430426,-5.4980852211

H,0,4.1768855947,4.6782371467,-3.8320132122

H,0,2.5606998315,4.5434295872,-6.3763950915

H,0,1.7799387547,2.8867732003,-6.1437161508

H,0,1.6990892512,5.2553373109,-4.1421096933

H,0,0.7332795716,2.3204068951,-3.9798192768

H,0,0.6998848563,3.577810767,-2.6166331063

Cation-B3LYP-D2/6-31+G/SMD- Conf2**

/home/bibaswanbiswas/c8/23parentSM2B3D2PSSMD

parent sm conf 2

B3LYP/6-31+G**

E(RB3LYP) = -519.597337906

Zero-point correction= 0.241141 (Hartree/Particle)

Thermal correction to Energy= 0.253568

Thermal correction to Enthalpy= 0.254512

Thermal correction to Gibbs Free Energy= 0.202903

Sum of electronic and ZPE= -519.356197

Sum of electronic and thermal Energies= -519.343770

Sum of electronic and thermal Enthalpies= -519.342826

Sum of electronic and thermal Free Energies= -519.394435

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.116	46.484	108.621

C,0,1.9652299496,-0.7576776524,-2.2301376274

O,0,2.7191617294,0.4747767898,-2.3948841081

C,0,2.8081880972,0.9569858241,-3.634762971

O,0,2.2983312928,0.4497493669,-4.6157030489

C,0,3.6576127806,2.2177503173,-3.5983559547

N,0,3.7297355644,2.9908131533,-4.8864470241

C,0,4.4474421771,2.2057474241,-5.951866044

C,0,4.5298375254,4.2356031967,-4.6039714402

C,0,2.3457687206,3.391687441,-5.4221243067

C,0,1.4766812339,4.0450285002,-4.3908107459

C,0,1.1749635428,5.3455589845,-4.4282959901

H,0,2.0515002563,-1.0054594181,-1.171937447

H,0,0.9203917538,-0.5909066241,-2.5055106667

H,0,2.3995100144,-1.546029421,-2.8504296121

H,0,4.683192749,1.9452617936,-3.3329201203

H,0,3.2696726655,2.8899373705,-2.8308600722

H,0,3.869962493,1.3120132798,-6.1801973191

H,0,4.5306783026,2.8469743007,-6.8308821646

H,0,5.4357990982,1.9474808987,-5.5679446359

H,0,5.5113016024,3.929059611,-4.2379770436

H,0,4.6202002532,4.7884754083,-5.5399544939

H,0,4.002864993,4.8270577279,-3.8550190432

H,0,2.553891519,4.0644522258,-6.2563156763

H,0,1.8976397655,2.4706158629,-5.7952538462

H,0,1.0616602318,3.4064626139,-3.6128291174

H,0,1.5781291902,5.9943253357,-5.2042088787

H,0,0.509684498,5.7915736888,-3.6927236023

23TS-B3LYP-D2/6-31+G/SMD**

/home/bibaswanbiswas/c8/23parentTSB3D2PSSMD

parent ts exo s-cis

B3LYP/6-31+G**

E(RB3LYP) = -519.072558527

Zero-point correction= 0.222269 (Hartree/Particle)

Thermal correction to Energy= 0.234857

Thermal correction to Enthalpy= 0.235801

Thermal correction to Gibbs Free Energy= 0.184387

Sum of electronic and ZPE= -518.850290

Sum of electronic and thermal Energies= -518.837702

Sum of electronic and thermal Enthalpies= -518.836758

Sum of electronic and thermal Free Energies= -518.888172

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.375	46.897	108.210

C,0,2.0047006433,-0.8044424496,-2.3027812513

O,0,2.7223329922,0.4308067966,-2.4448726789

C,0,2.8250386391,0.9210915309,-3.7257297696

C,0,3.4698023078,2.195292889,-3.7248377997

N,0,3.8248851462,2.8827287127,-4.8658770729

C,0,4.6876410956,4.0461349009,-4.5814234795

O,0,2.3817504562,0.2863329757,-4.6933860752

C,0,4.2996464335,2.1313068673,-6.0464092197

C,0,2.1150828813,3.8617237312,-5.7001923815

C,0,1.5065625233,4.2444559579,-4.4914824762

C,0,0.980783541,3.2908918565,-3.6557957296

H,0,2.0155143257,-1.0288804528,-1.233567435

H,0,0.972228135,-0.6999567944,-2.6542847811

H,0,2.493764266,-1.6105009566,-2.8605698226

H,0,3.6950459969,2.6663354068,-2.7791447584

H,0,5.2868150687,1.702905752,-5.8302246142

H,0,3.5931649333,1.3375478348,-6.2791417453

H,0,4.3764138849,2.8303024677,-6.882679289

H,0,5.6617348028,3.7025672889,-4.2109068464

H,0,4.8213962455,4.6190800748,-5.5009685801

H,0,4.2048760121,4.6703042568,-3.8259319766

H,0,2.596238814,4.5964911963,-6.3398643345

H,0,1.7928345587,2.9419085709,-6.181218657

H,0,1.6976132136,5.2446907347,-4.1041401342

H,0,0.7223176116,2.3072313445,-4.0358289341

H,0,0.666069472,3.5311105068,-2.6427801572

Cation-B3LYP-D2/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/23parentSM2B3D2SB

parent sm conf 2

B3LYP/6-31G*

E(RB3LYP) = -519.541373957

Zero-point correction= 0.241730 (Hartree/Particle)

Thermal correction to Energy= 0.254499

Thermal correction to Enthalpy= 0.255443

Thermal correction to Gibbs Free Energy= 0.202324

Sum of electronic and ZPE= -519.299644

Sum of electronic and thermal Energies= -519.286875

Sum of electronic and thermal Enthalpies= -519.285931

Sum of electronic and thermal Free Energies= -519.339050

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.700	46.763	111.799

C,0,2.0243629283,-0.7919080244,-2.2532833654

O,0,2.7865949024,0.4330936219,-2.4083864972

C,0,2.7742877251,0.9772892654,-3.6200782967

O,0,2.1850063012,0.5363730471,-4.5857022996

C,0,3.6207421924,2.2452729313,-3.5782449206

N,0,3.718982322,2.9936657208,-4.8805131823

C,0,4.4358884884,2.1676470057,-5.9167961407

C,0,4.5225235898,4.2396631444,-4.61375006

C,0,2.3385479335,3.3982601218,-5.4408425062

C,0,1.4630752774,4.0570420179,-4.4204755028

C,0,1.2142232602,5.3679051105,-4.4239187567

H,0,2.1579475357,-1.080101455,-1.2111692032

H,0,0.9719319468,-0.6007525211,-2.4773958608

H,0,2.41699461,-1.5573123315,-2.9273357987

H,0,4.638639665,1.9888257822,-3.2746497115

H,0,3.2069849686,2.9282178087,-2.8331775015

H,0,3.8570524605,1.2632673551,-6.0940689131

H,0,4.5109777888,2.7649224879,-6.8268371347

H,0,5.4299225686,1.9305180136,-5.533676887

H,0,5.4903541367,3.9443468,-4.2061510355

H,0,4.6502481141,4.7657823415,-5.5604773496

H,0,3.9721276092,4.8580055828,-3.9044522122

H,0,2.5634055344,4.066681194,-6.274408239

H,0,1.8980254641,2.4744889463,-5.813547338

H,0,0.9947672537,3.4102274423,-3.6818089634

H,0,1.6569712279,6.0269948416,-5.1680718871

H,0,0.5484461949,5.818901749,-3.6931034369

23TS-B3LYP-D2/6-31G*/PCM

/home/bibaswanbiswas/c8/23parentTSB3D2SB

parent ts exo s-cis

B3LYP/6-31G*

E(RB3LYP) = -519.022559562

Zero-point correction= 0.223787 (Hartree/Particle)

Thermal correction to Energy= 0.236342

Thermal correction to Enthalpy= 0.237286

Thermal correction to Gibbs Free Energy= 0.185854

Sum of electronic and ZPE= -518.798772

Sum of electronic and thermal Energies= -518.786218

Sum of electronic and thermal Enthalpies= -518.785274

Sum of electronic and thermal Free Energies= -518.836705

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.307	46.624	108.247

C,0,1.9843757471,-0.8034079907,-2.3643243653

O,0,2.7307391171,0.4134089273,-2.4657521081

C,0,2.8096974076,0.945246613,-3.7311581953

C,0,3.4878519713,2.1975602465,-3.7105020712

N,0,3.8269269367,2.8868606111,-4.8594447179

C,0,4.6584119928,4.071458751,-4.5795224612

O,0,2.3066530007,0.3685880326,-4.704942114

C,0,4.3365020156,2.1240427835,-6.0182498556

C,0,2.1024227713,3.7817537401,-5.6952845874

C,0,1.5169264324,4.2362596519,-4.5009781803

C,0,1.0291738374,3.3279082169,-3.598679955

H,0,2.0220684802,-1.0861628422,-1.309787578

H,0,0.9452793347,-0.653842764,-2.6791114033

H,0,2.4289344341,-1.5900157111,-2.9839381066

H,0,3.7631122529,2.6400654658,-2.7647416184

H,0,5.3544193251,1.7739007678,-5.804666378

H,0,3.6774184051,1.2768582475,-6.1968671913

H,0,4.3490289584,2.7888828793,-6.8861763019

H,0,5.6300244127,3.7579773144,-4.17777547

H,0,4.8017611419,4.6309970071,-5.5063798537

H,0,4.1387078033,4.696721384,-3.8496608805

H,0,2.5380164213,4.4775663103,-6.407621438

H,0,1.7833959454,2.8241047057,-6.0983269923

H,0,1.6995427905,5.2628150226,-4.1851439828

H,0,0.7583996453,2.3280805473,-3.9213617993

H,0,0.7344634195,3.6198330823,-2.5936423947

Cation- B97D3/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/23parentSM2B97D3SB

parent sm conf 2

B97D3/6-31G*

E(RB97D3) = -519.191750743

Zero-point correction= 0.236901 (Hartree/Particle)

Thermal correction to Energy= 0.250194

Thermal correction to Enthalpy= 0.251138

Thermal correction to Gibbs Free Energy= 0.195480

Sum of electronic and ZPE= -518.954849

Sum of electronic and thermal Energies= -518.941557

Sum of electronic and thermal Enthalpies= -518.940613

Sum of electronic and thermal Free Energies= -518.996271

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	156.999	48.119	117.141

C,0,2.0042759519,-0.7911685801,-2.2412586973

O,0,2.7740178964,0.4378099713,-2.3982410602

C,0,2.7776478474,0.9709418054,-3.6257601666

O,0,2.1969883869,0.519494911,-4.5995173743

C,0,3.633958441,2.2378787468,-3.5811881665

N,0,3.7312430636,2.9955367457,-4.8858949575

C,0,4.4478815717,2.1697209954,-5.9320615865

C,0,4.5347943146,4.2478514305,-4.6144459299

C,0,2.3354667853,3.4004931123,-5.441423949

C,0,1.4565518808,4.0521133877,-4.4197235059

C,0,1.1987194767,5.3684893689,-4.4123603823

H,0,2.1290581285,-1.0672984918,-1.1920547565

H,0,0.9513580469,-0.6005242497,-2.4759353852

H,0,2.4049419549,-1.566458843,-2.9033720178

H,0,4.6542875579,1.9739709335,-3.2818270149

H,0,3.2310555842,2.9233363011,-2.8286549375

H,0,3.8771923192,1.2557677551,-6.1005990344

H,0,4.507796255,2.7626858602,-6.8487273253

H,0,5.4512428216,1.9422317603,-5.5610986783

H,0,5.5055058746,3.9558770083,-4.2051888711

H,0,4.6652568706,4.7807589795,-5.5596903036

H,0,3.9842397167,4.8663513133,-3.9018265372

H,0,2.5557241328,4.0695503358,-6.2791618221

H,0,1.8999666847,2.4710823837,-5.8151320446

H,0,0.9752558793,3.3969564072,-3.6909505946

H,0,1.6440167083,6.0445183113,-5.1447170516

H,0,0.5205878483,5.8093503401,-3.6815108497

23TS-B97D3/6-31G*/PCM

/home/bibaswanbiswas/c8/23parentTSB97D3SB

parent ts exo s-cis

B97D3/6-31G*

E(RB97D3) = -518.682459365

Zero-point correction= 0.219801 (Hartree/Particle)

Thermal correction to Energy= 0.232694

Thermal correction to Enthalpy= 0.233638

Thermal correction to Gibbs Free Energy= 0.181304

Sum of electronic and ZPE= -518.462658

Sum of electronic and thermal Energies= -518.449766

Sum of electronic and thermal Enthalpies= -518.448821

Sum of electronic and thermal Free Energies= -518.501156

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 146.018 47.627 110.147

C,0,1.9722204471,-0.8322814371,-2.4121711006

O,0,2.7705079801,0.357220501,-2.4877427541

C,0,2.8539075202,0.9258429356,-3.7589447894

C,0,3.5996165478,2.1303188479,-3.7198191189

N,0,3.8194815775,2.8955481491,-4.8789616287

C,0,4.6408325521,4.0983482248,-4.5813615223

O,0,2.3103217465,0.3842120786,-4.7439941134

C,0,4.3781528455,2.1483239159,-6.0427935664

C,0,2.1687044161,3.6346017954,-5.6164317138

C,0,1.5209910736,4.2356721414,-4.4871209724

C,0,0.9217624491,3.4722984756,-3.531015571

H,0,2.0179892921,-1.1498693168,-1.3642987778

H,0,0.9286933003,-0.6333096339,-2.6972962359

H,0,2.3685221455,-1.6249658855,-3.0626226966

H,0,3.8254037636,2.606513305,-2.7733437701

H,0,5.4083782138,1.8496519685,-5.8088559396

H,0,3.7568915622,1.2665967564,-6.2083882364

H,0,4.3673981207,2.8020214128,-6.9223693936

H,0,5.6251037691,3.7820886839,-4.212113127

H,0,4.7543243993,4.6904572714,-5.4947273812

H,0,4.1292969331,4.6895598214,-3.8155947259

H,0,2.539553277,4.2778096085,-6.4165611057

H,0,1.786204829,2.6691221013,-5.9495841057

H,0,1.6803160319,5.3020213369,-4.3053690641

H,0,0.7182292755,2.416476807,-3.7030422702

H,0,0.5514499315,3.9031811348,-2.5995163189

Cation- N12/6-31+G/PCM- Conf2**

/home/bibaswanbiswas/c8/SM2N12PS

parent sm conf 2

N12/6-31+G**

E(RN12) = -519.407692482

Zero-point correction= 0.239843 (Hartree/Particle)

Thermal correction to Energy= 0.252803

Thermal correction to Enthalpy= 0.253747

Thermal correction to Gibbs Free Energy= 0.200521

Sum of electronic and ZPE= -519.167849

Sum of electronic and thermal Energies= -519.154890

Sum of electronic and thermal Enthalpies= -519.153946

Sum of electronic and thermal Free Energies= -519.207171

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 158.636 47.526 112.022

C,0,2.0714897046,-0.8407639046,-2.278635364

O,0,2.8061443038,0.3809669936,-2.4360077855

C,0,2.7841441775,0.9515683637,-3.6250072628

O,0,2.197845739,0.5217250676,-4.5931266227

C,0,3.6083228695,2.2214214517,-3.5681294851

N,0,3.7084720776,2.9884326525,-4.8476454746

C,0,4.4013331225,2.1769631405,-5.8962885868

C,0,4.5250163173,4.2090616707,-4.5669291908

C,0,2.3370813691,3.4134397705,-5.3862965157

C,0,1.5015609048,4.1598724426,-4.4087141007

C,0,1.1836219568,5.4466550772,-4.5541788526

H,0,2.2858131899,-1.1787829447,-1.2736502

H,0,1.0102003001,-0.6483610188,-2.4000719657

H,0,2.403662779,-1.5701009203,-3.0099766184

H,0,4.6183901086,1.9680291858,-3.258710985

H,0,3.1948740705,2.8808673488,-2.8112371498

H,0,3.8087995797,1.2968792137,-6.1038119037

H,0,4.5006994773,2.7852703672,-6.7869276516

H,0,5.3813899821,1.900894284,-5.525776302

H,0,5.4887801052,3.9049370402,-4.1774055223

H,0,4.6539570844,4.755006705,-5.4932924566

H,0,4.0018602117,4.8228192993,-3.8447370689

H,0,2.5533508306,4.0133724244,-6.2638879686

H,0,1.8569245547,2.490595542,-5.6933491202

H,0,1.0795916867,3.5989804781,-3.5854786464

H,0,1.560506309,6.0374948172,-5.3774838229

H,0,0.5251991879,5.940073452,-3.8555663769

23TS-N12/6-31+G/PCM**

/home/bibaswanbiswas/c8/TSparentN12PS

parent ts exo s-cis

N12/6-31+G**

E(RN12) = -518.906645363

Zero-point correction= 0.222212 (Hartree/Particle)

Thermal correction to Energy= 0.235111

Thermal correction to Enthalpy= 0.236056

Thermal correction to Gibbs Free Energy= 0.183660

Sum of electronic and ZPE= -518.684434

Sum of electronic and thermal Energies= -518.671534

Sum of electronic and thermal Enthalpies= -518.670590

Sum of electronic and thermal Free Energies= -518.722986

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.535	47.424	110.277

C,0,2.0564008038,-0.8340301518,-2.3495362104

O,0,2.7287859217,0.4062835961,-2.4739485019

C,0,2.8263414038,0.9218125193,-3.7355218924

C,0,3.4729672503,2.181442418,-3.7220999019

N,0,3.8072613303,2.8830164302,-4.8602357181

C,0,4.677762835,4.026476963,-4.5687300017

O,0,2.3752374237,0.3057777503,-4.7075628004

C,0,4.2881451469,2.1203505386,-6.0194213949

C,0,2.1462231716,3.8139069453,-5.6733577565

C,0,1.5140854742,4.2812450804,-4.5061997931

C,0,0.9207867272,3.4148730948,-3.6379747183

H,0,2.0712070404,-1.0756361934,-1.2925712064

H,0,1.0281920944,-0.7604798853,-2.6973355961

H,0,2.5630659969,-1.6139310063,-2.9142890342

H,0,3.6975392974,2.6442133067,-2.779456683

H,0,5.2852642597,1.7358334363,-5.8092057777

H,0,3.6128424516,1.2960694277,-6.2054322792

H,0,4.3298500079,2.778161461,-6.8810952093

H,0,5.6385700062,3.6730395143,-4.1978580289

H,0,4.827826628,4.6044523189,-5.4731464904

H,0,4.2087779928,4.6498873853,-3.8157224017

H,0,2.5974444757,4.5107521758,-6.3650518242

H,0,1.7951344597,2.8900081198,-6.1098752419

H,0,1.6945670388,5.3017385352,-4.1919454324

H,0,0.6748726773,2.4089171092,-3.9410302632

H,0,0.5751020847,3.7332801107,-2.6654358417

23TS-UN12/6-31+G/PCM**

/home/bibaswanbiswas/c8/TSparentUN12PS

parent ts exo s-cis

UN12/6-31+G**

E(UN12) = -518.906645392

Zero-point correction= 0.222211 (Hartree/Particle)

Thermal correction to Energy= 0.235110

Thermal correction to Enthalpy= 0.236054

Thermal correction to Gibbs Free Energy= 0.183663

Sum of electronic and ZPE= -518.684434

Sum of electronic and thermal Energies= -518.671535

Sum of electronic and thermal Enthalpies= -518.670591

Sum of electronic and thermal Free Energies= -518.722982

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.534	47.424	110.266

C,0,2.0562314234,-0.8341384674,-2.3498227891

O,0,2.7286613326,0.4061597084,-2.4741656537

C,0,2.8263266439,0.9217465195,-3.7356962028

C,0,3.4729797542,2.1813736915,-3.7221539334

N,0,3.8073909481,2.8829435016,-4.8602371409

C,0,4.6775922754,4.0266049027,-4.5686980878

O,0,2.3752718239,0.3058070456,-4.7078170781

C,0,4.288440442,2.1203760863,-6.0194046535

C,0,2.1459508533,3.8135091356,-5.6734184022

C,0,1.5141907307,4.2812295883,-4.5062240298

C,0,0.9210695462,3.4152829918,-3.6374100435

H,0,2.0707044697,-1.0756102683,-1.2928223807

H,0,1.0281333471,-0.7606277306,-2.6979488943

H,0,2.563079461,-1.6141210139,-2.9142986382

H,0,3.6974605392,2.6441013723,-2.7794656866

H,0,5.2856799214,1.7361397345,-5.8092301366

H,0,3.6133543312,1.2959067796,-6.2053758607

H,0,4.3299274535,2.7781636975,-6.8811061874

H,0,5.6383788873,3.6734245838,-4.1975216571

H,0,4.8277681153,4.6044599978,-5.4731742116

H,0,4.2082992147,4.6500536269,-3.8159120456

H,0,2.5969682721,4.5101282547,-6.3654700719

H,0,1.795007477,2.8892884731,-6.1093693893

H,0,1.6946548337,5.3018860171,-4.1924755237

H,0,0.67512946,2.4091485921,-3.9398543473

H,0,0.5756024434,3.7342241793,-2.6649669541

Cation- M06/6-31+G/PCM- Conf2**

/home/bibaswanbiswas/c8/23SMcatUm06pcmdmf

M06/6-31+G**

E(RM06) = -519.181390021

Zero-point correction= 0.239598 (Hartree/Particle)

Thermal correction to Energy= 0.252131

Thermal correction to Enthalpy= 0.253075

Thermal correction to Gibbs Free Energy= 0.201601

Sum of electronic and ZPE= -518.941792

Sum of electronic and thermal Energies= -518.929259

Sum of electronic and thermal Enthalpies= -518.928315

Sum of electronic and thermal Free Energies= -518.979789

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.215	47.047	108.338

C,0,1.8449022255,-0.6202354751,-2.2587965391

O,0,2.653549298,0.5596326055,-2.4164482523

C,0,2.857624907,0.9670456834,-3.6584316879

O,0,2.4207786733,0.4291083116,-4.6513663997

C,0,3.7298770733,2.2021951378,-3.6229354871

N,0,3.7738587923,2.9876199218,-4.8983089406

C,0,4.4871082033,2.2251543877,-5.9774959624

C,0,4.554317142,4.2395541458,-4.6232107253

C,0,1.4967903942,3.9349821651,-4.347557834

C,0,0.3973762362,3.3146767553,-3.9191606785

C,0,2.371657725,3.352501454,-5.4033239894

H,0,1.7950352201,-0.8002957435,-1.1866052159

H,0,0.8466544672,-0.4403973485,-2.6656713981

H,0,2.3095351457,-1.4658326142,-2.7706623205

H,0,4.7567850783,1.9060896296,-3.3796511894

H,0,5.5049191822,2.0197199265,-5.6399798894

H,0,3.9496886874,1.2975544823,-6.1692918168

H,0,4.5101386922,2.8487580723,-6.8731071551

H,0,5.5521526301,3.9593235055,-4.2798093552

H,0,4.6257713577,4.8119159739,-5.5496004358

H,0,4.0510064231,4.826123165,-3.8540617691

H,0,2.5491791786,4.0508354476,-6.2288188021

H,0,1.9436244956,2.4320776298,-5.8065152052

H,0,1.7534193863,4.9189327707,-3.9546863359

H,0,0.1014380287,2.3414406104,-4.31048681

H,0,-0.2530567785,3.7660907643,-3.1754353262

H,0,3.3787311354,2.8610796355,-2.823552479

23TS- UM06/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/23TSUm06pcmdmf

experimental system pcm m06 +G**

UM06/6-31+G**

E(UM06) = -518.672218948

Zero-point correction= 0.221418 (Hartree/Particle)

Thermal correction to Energy= 0.234072

Thermal correction to Enthalpy= 0.235017

Thermal correction to Gibbs Free Energy= 0.183563

Sum of electronic and ZPE= -518.450801

Sum of electronic and thermal Energies= -518.438147

Sum of electronic and thermal Enthalpies= -518.437202

Sum of electronic and thermal Free Energies= -518.488656

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	146.883	47.194	108.292

C,0,1.970228096,-0.746171725,-2.320652426

O,0,2.7138886572,0.4578462826,-2.4575862697

C,0,2.8455666321,0.9308357404,-3.7323189364

C,0,3.4750871328,2.2082126603,-3.7315061733

N,0,3.8255321724,2.8921291851,-4.8748804425

C,0,4.6848178613,4.0477189436,-4.5897630335

O,0,2.422951473,0.289275982,-4.6973658933

C,0,4.3125034756,2.1383997425,-6.0399849742

C,0,2.0899516843,3.8451866391,-5.6893655938

C,0,1.5027604756,4.2015719264,-4.4714539513

C,0,1.0274548926,3.2271183222,-3.6348624496

H,0,1.9503834857,-0.968129213,-1.2527113365

H,0,0.9480044431,-0.6177236985,-2.6934686426

H,0,2.4440512586,-1.5707451583,-2.8626157051

H,0,3.7147174459,2.6699841627,-2.7806019011

H,0,5.3173399979,1.7474151076,-5.8312025334

H,0,3.6363019858,1.3112599221,-6.2516785084

H,0,4.3589887852,2.8154107868,-6.8981176418

H,0,5.6588210654,3.7065763073,-4.2148460994

H,0,4.8306540664,4.6278022282,-5.5045978175

H,0,4.2073777777,4.678309554,-3.8347120819

H,0,2.5283754223,4.5944440246,-6.346482319

H,0,1.7864105014,2.9145992827,-6.1679192638

H,0,1.6720213918,5.2058035996,-4.0797160053

H,0,0.755815771,2.2487220285,-4.0258098728

H,0,0.7342480491,3.4416083664,-2.6098201275

23TS- UM06/6-31+G/PCM(water)**

/home/bibaswanbiswas/c8/Parentcalcs/23TSUm06pcmwater

E(UM06) = -518.672476705

Zero-point correction= 0.221405 (Hartree/Particle)

Thermal correction to Energy= 0.234061

Thermal correction to Enthalpy= 0.235005

Thermal correction to Gibbs Free Energy= 0.183546

Sum of electronic and ZPE= -518.451072

Sum of electronic and thermal Energies= -518.438415

Sum of electronic and thermal Enthalpies= -518.437471

Sum of electronic and thermal Free Energies= -518.488931

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	146.876	47.199	108.306

C,0,1.9695982163,-0.7456296158,-2.3200625243

O,0,2.7138787945,0.458026488,-2.4576400498

C,0,2.8456119394,0.9308025184,-3.7324546517

C,0,3.4748567005,2.2082544201,-3.7319115827

N,0,3.8260580792,2.8919919096,-4.875004415

C,0,4.6850540651,4.047828855,-4.589717002

O,0,2.4232401792,0.2886829825,-4.6974095327

C,0,4.3129521465,2.1386576628,-6.0403414965

C,0,2.0888615652,3.8458551643,-5.6898126723

C,0,1.5026418738,4.2009711333,-4.4712638065

C,0,1.0280720924,3.2257012984,-3.6349517392

H,0,1.9492396739,-0.9667984534,-1.2519863915

H,0,0.9475357382,-0.6169374533,-2.6932184318

H,0,2.4433635847,-1.5708502445,-2.8610861372

H,0,3.7145771741,2.6699108704,-2.7809550357

H,0,5.3176407955,1.7472479549,-5.8316257564

H,0,3.6365150123,1.3119332834,-6.2527967969

H,0,4.3599499113,2.816046309,-6.8981076807

H,0,5.6592330041,3.706879193,-4.2151066235

H,0,4.8305212448,4.6281405267,-5.5044306738

H,0,4.2075693702,4.6781270889,-3.8344759477

H,0,2.5275237628,4.5954535382,-6.3463272911

H,0,1.7862144645,2.9151140826,-6.1686400452

H,0,1.672315304,5.2048026211,-4.0786978187

H,0,0.7556070662,2.2477520294,-4.0264786104

H,0,0.7356222414,3.4394968371,-2.6095372863

Cation- M052X/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/m052x/m052xsm

sean allyl ester starting material for m05 isotope effects

M052X/6-31+G**

E(RM052X) = -519.458425931

Zero-point correction= 0.244429 (Hartree/Particle)

Thermal correction to Energy= 0.257198

Thermal correction to Enthalpy= 0.258142

Thermal correction to Gibbs Free Energy= 0.205418

Sum of electronic and ZPE= -519.213997

Sum of electronic and thermal Energies= -519.201228

Sum of electronic and thermal Enthalpies= -519.200284

Sum of electronic and thermal Free Energies= -519.253008

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.394	46.517	110.968

C,0,1.8753927368,-0.653356482,-2.262116733

O,0,2.6767889894,0.5449787039,-2.4048214272

C,0,2.8302734595,0.9920222651,-3.6396703478

O,0,2.3491328009,0.4808431155,-4.6262806566

C,0,3.7148547103,2.2236890973,-3.6109402379

N,0,3.7695804993,2.9878272364,-4.8947924428

C,0,4.4782688998,2.2046598567,-5.9610553401

C,0,4.5598708111,4.2352989127,-4.6289714907

C,0,1.499947069,3.9470141828,-4.3501513435

C,0,0.3904728638,3.3291856057,-3.9460576201

C,0,2.3824597572,3.3621705081,-5.4110058485

H,0,1.8880661532,-0.8770341196,-1.2017770858

H,0,0.8643990353,-0.452480746,-2.6082148757

H,0,2.3222353929,-1.458958433,-2.8393002029

H,0,4.7316239643,1.9170587925,-3.3622916506

H,0,5.4904488518,2.0014301033,-5.6199114776

H,0,3.9338930029,1.2829623267,-6.1351936011

H,0,4.5007743534,2.8155189657,-6.8601434295

H,0,5.5430234999,3.9479595132,-4.2642886778

H,0,4.6503681149,4.7843921539,-5.5622165124

H,0,4.0450051088,4.8336595975,-3.8832143747

H,0,2.5659723758,4.0694651792,-6.2202136068

H,0,1.9492889221,2.4527716061,-5.8173098904

H,0,1.7575595144,4.9201196944,-3.9459236071

H,0,0.0994333919,2.3664758427,-4.3527727895

H,0,-0.2611987378,3.7786427279,-3.2077648691

H,0,3.3549274594,2.8893347933,-2.828571861

23TS- M052X/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/m052x/m052xts

sean allyl ester trying to kill m052x

M052X/6-31+G**

E(RM052X) = -518.943406641

Zero-point correction= 0.227481 (Hartree/Particle)

Thermal correction to Energy= 0.239713

Thermal correction to Enthalpy= 0.240657

Thermal correction to Gibbs Free Energy= 0.189859

Sum of electronic and ZPE= -518.715925

Sum of electronic and thermal Energies= -518.703694

Sum of electronic and thermal Enthalpies= -518.702749

Sum of electronic and thermal Free Energies= -518.753548

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	150.422	45.488	106.914

C,0,2.0214222998,-0.801470997,-2.3436663695

O,0,2.6920040321,0.4592246856,-2.4613388313

C,0,2.7699657924,0.9663735427,-3.7242952189

C,0,3.3442741961,2.2701939876,-3.7241876718

N,0,3.7411570132,2.9195768418,-4.8868343303

C,0,4.6309569671,4.0525916432,-4.5786546222

O,0,2.3202534765,0.3379528755,-4.6871908685

C,0,4.2760879426,2.1201346678,-6.0058787783

C,0,2.1512261715,3.8242141753,-5.6936255173

C,0,1.5332829504,4.2552068717,-4.5079695332

C,0,1.1363014059,3.2610890069,-3.6419244858

H,0,2.0412077778,-1.0429547931,-1.2849102024

H,0,0.9936515017,-0.7206055204,-2.6955861613

H,0,2.5426923356,-1.5662803349,-2.9173733919

H,0,3.6824212148,2.6797841947,-2.7863429004

H,0,5.2570505295,1.7243886643,-5.7348663684

H,0,3.5946863008,1.3061616519,-6.2243960353

H,0,4.371574235,2.7754799723,-6.8710644165

H,0,5.5631239473,3.6804056233,-4.1484891814

H,0,4.8385835963,4.6010428524,-5.4953510396

H,0,4.1321954646,4.7057433756,-3.864886474

H,0,2.593910139,4.5369841137,-6.3821675512

H,0,1.7929387797,2.9053817144,-6.1481182601

H,0,1.7310244274,5.2547601481,-4.1349016844

H,0,0.7878394384,2.3144676581,-4.0377774451

H,0,0.8744220644,3.4776153786,-2.6122436608

Cation M062X/6-31+G/PCM Conf1**

/home/bibaswanbiswas/c8/Parentcalcs/23parentSM1m062xSSpcm

try at new ts's with small basis

m062X/6-31+G**

E(RM062X) = -519.293599561

Zero-point correction= 0.242639 (Hartree/Particle)

Thermal correction to Energy= 0.255413

Thermal correction to Enthalpy= 0.256357

Thermal correction to Gibbs Free Energy= 0.203557

Sum of electronic and ZPE= -519.050961

Sum of electronic and thermal Energies= -519.038186

Sum of electronic and thermal Enthalpies= -519.037242

Sum of electronic and thermal Free Energies= -519.090042

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.274	46.678	111.128

C,0,1.849223013,-0.6188169651,-2.2621308349

O,0,2.6606202547,0.5626727661,-2.4077677231

C,0,2.8234429286,1.0062399898,-3.6431787688

O,0,2.3379450616,0.5038532678,-4.6307662106

C,0,3.728264934,2.2252443523,-3.6144898326

N,0,3.7798387297,2.9935116574,-4.8997112637

C,0,4.4832181769,2.2061944663,-5.9685684755

C,0,4.5685749377,4.2446351055,-4.6367230942

C,0,1.4976765687,3.9134462822,-4.3335105962

C,0,0.4007832547,3.2710286601,-3.9320590757

C,0,2.3855731262,3.3664405391,-5.4092690223

H,0,1.8434744057,-0.8343517523,-1.1970046035

H,0,0.8402812973,-0.4164012566,-2.6237104802

H,0,2.2917964463,-1.4420646717,-2.8240002122

H,0,4.745515658,1.9040693351,-3.3753778555

H,0,5.5018987492,2.0079858558,-5.6358763057

H,0,3.9401671153,1.2783279732,-6.1324475844

H,0,4.495741449,2.810415033,-6.8754548565

H,0,5.551809646,3.9627077119,-4.2606424563

H,0,4.666990662,4.7897545742,-5.5743289395

H,0,4.0459267708,4.8505843838,-3.8983638166

H,0,2.5623699749,4.0959254757,-6.2038299793

H,0,1.963114415,2.4603281426,-5.8410394482

H,0,1.7473061035,4.8825532228,-3.9069911153

H,0,0.1178975948,2.3101716648,-4.3563570069

H,0,-0.252243492,3.6958757141,-3.1770532778

H,0,3.3856552185,2.8953194721,-2.8243191645

Cation- M062X/6-31+G/PCM-Conf2**

/home/bibaswanbiswas/c8/Parentcalcs/23parentSM2M062XSS

parent sm

M062X/6-31+G**

E(RM062X) = -519.292775633

Zero-point correction= 0.243092 (Hartree/Particle)

Thermal correction to Energy= 0.255685

Thermal correction to Enthalpy= 0.256630

Thermal correction to Gibbs Free Energy= 0.204183

Sum of electronic and ZPE= -519.049683

Sum of electronic and thermal Energies= -519.037090

Sum of electronic and thermal Enthalpies= -519.036146

Sum of electronic and thermal Free Energies= -519.088593

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.445	46.378	110.383

C,0,1.9991012581,-0.7446404209,-2.259699165

O,0,2.7746449214,0.4608314914,-2.4080355116

C,0,2.7764752357,1.0065000642,-3.6126826673

O,0,2.1822035176,0.5747384982,-4.5733649137

C,0,3.6397917839,2.2561533747,-3.584392107

N,0,3.7300377836,2.9918314704,-4.8856522347

C,0,4.439955203,2.1636346937,-5.9178217952

C,0,4.5370394966,4.232044221,-4.6275557578

C,0,2.3611652444,3.395750662,-5.4427532979

C,0,1.462128603,4.0088496952,-4.4135005246

C,0,1.1851919223,5.3118105524,-4.3865830858

H,0,2.1220664504,-1.0398098054,-1.2211170058

H,0,0.9524227288,-0.5370376996,-2.4844292693

H,0,2.3829650687,-1.513323233,-2.9311899834

H,0,4.6539311343,1.9758130129,-3.2894278981

H,0,3.2478346394,2.9416301204,-2.829403239

H,0,3.8702886525,1.2534151264,-6.0908343918

H,0,4.5045099774,2.75058318,-6.8338843052

H,0,5.4393070758,1.9341326502,-5.5481511672

H,0,5.5039437003,3.9387332156,-4.2200863163

H,0,4.669180799,4.7562160329,-5.5732038185

H,0,3.9979384042,4.8593576785,-3.9186506606

H,0,2.579477771,4.0993142796,-6.2488226153

H,0,1.9273193218,2.4880766755,-5.8604652531

H,0,0.9839517466,3.3369971895,-3.7033204504

H,0,1.6276870289,6.0008534451,-5.1021136848

H,0,0.498472531,5.724861829,-3.6551818808

TS M062X/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/23iparentTSm062xpcmSS

try at new ts's with small basis

m062X/6-31+G**

E(RM062X) = -518.778953134

Zero-point correction= 0.225580 (Hartree/Particle)

Thermal correction to Energy= 0.237903

Thermal correction to Enthalpy= 0.238847

Thermal correction to Gibbs Free Energy= 0.187871

Sum of electronic and ZPE= -518.553373

Sum of electronic and thermal Energies= -518.541050

Sum of electronic and thermal Enthalpies= -518.540106

Sum of electronic and thermal Free Energies= -518.591082

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.286	45.846	107.287

C,0,2.0079655936,-0.7935153283,-2.3536069007

O,0,2.6975626855,0.4497499733,-2.4681593401

C,0,2.7778222507,0.9662920821,-3.7264353507

C,0,3.3727023027,2.2636023109,-3.7181223987

N,0,3.7608795511,2.9160434216,-4.8795746054

C,0,4.635873307,4.0629593683,-4.5812225016

O,0,2.3169154317,0.3566302452,-4.6938582812

C,0,4.2912041559,2.1186818033,-6.0026370172

C,0,2.1363527999,3.8099041901,-5.6957164935

C,0,1.5289269331,4.2407474105,-4.5064796523

C,0,1.126822727,3.2624229175,-3.6269326029

H,0,2.0431572378,-1.0544553011,-1.2969439024

H,0,0.9707950185,-0.6914397995,-2.6824126833

H,0,2.4992479247,-1.5659040525,-2.9495537368

H,0,3.7050144967,2.6764631329,-2.7768767993

H,0,5.2776284891,1.7243438741,-5.7381170746

H,0,3.610329159,1.2997941286,-6.2185802697

H,0,4.380961365,2.7729776131,-6.8722610405

H,0,5.580107906,3.708171632,-4.1558620402

H,0,4.8297675761,4.6153519924,-5.501526219

H,0,4.1319340065,4.7128595861,-3.8637747667

H,0,2.5720906557,4.5224305677,-6.3927925744

H,0,1.7923420512,2.877502255,-6.140222008

H,0,1.7149338327,5.2506948297,-4.1477159113

H,0,0.7912029524,2.301032558,-4.0057355428

H,0,0.8617135905,3.494119589,-2.5989202865

Cation- SOGGA11/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMSOGGA11gasSB

parent sm conf 2

SOGGA11/6-31G*

E(RSOGGA11) = -519.439679577

C,0,1.9798202338,-0.7762095285,-2.2151157052

O,0,2.7012436396,0.4541253901,-2.4094230064

C,0,2.8049988195,0.9064345208,-3.6526952863

O,0,2.3280223489,0.4111642095,-4.6483309619

C,0,3.6741118238,2.1728556777,-3.6024352308

N,0,3.741949616,2.9881076067,-4.8738456249

C,0,4.4274303364,2.216056744,-5.972857282

C,0,4.5616349058,4.2144008088,-4.5739155584

C,0,2.3385523732,3.424649043,-5.3860290314

C,0,1.4815267505,4.1171740421,-4.3803295744

C,0,1.1285978751,5.4017673622,-4.4730298394

H,0,1.9783252877,-0.9482402721,-1.1375477318

H,0,0.9566560721,-0.6839083377,-2.5916467598

H,0,2.4831241533,-1.598479862,-2.733242176

H,0,4.7008419712,1.8877787259,-3.3542242628

H,0,3.3160655034,2.8286588484,-2.8090057388

H,0,3.846796158,1.3225896996,-6.1922948711

H,0,4.4927388035,2.8575083045,-6.8530397177

H,0,5.431270583,1.9489071086,-5.6367165869

H,0,5.537320105,3.9050603396,-4.1952521109

H,0,4.6876263947,4.7815176563,-5.4974539013

H,0,4.0394286412,4.8210611381,-3.8347454116

H,0,2.5488466981,4.0692033288,-6.2411470881

H,0,1.8747456118,2.5024995474,-5.7372046811

H,0,1.0606175198,3.5040745793,-3.5857543603

H,0,1.4890386175,6.047239101,-5.2722683568

H,0,0.437701157,5.8513222178,-3.7627721441

Zero-point correction= 0.238319 (Hartree/Particle)

Thermal correction to Energy= 0.251473

Thermal correction to Enthalpy= 0.252417

Thermal correction to Gibbs Free Energy= 0.198953

Sum of electronic and ZPE= -519.201361

Sum of electronic and thermal Energies= -519.188207

Sum of electronic and thermal Enthalpies= -519.187262

Sum of electronic and thermal Free Energies= -519.240726

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	157.802	48.044	112.524

TS- SOGGA11/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSSOGGA11gasSB

parent ts exo s-cis

SOGGA11/6-31G*

E(RSOGGA11) = -518.995048971

Zero-point correction= 0.221969 (Hartree/Particle)

Thermal correction to Energy= 0.234854

Thermal correction to Enthalpy= 0.235798

Thermal correction to Gibbs Free Energy= 0.183306

Sum of electronic and ZPE= -518.773080

Sum of electronic and thermal Energies= -518.760195

Sum of electronic and thermal Enthalpies= -518.759251

Sum of electronic and thermal Free Energies= -518.811743

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.373	47.269	110.480

C,0,2.0668125601,-0.8699958378,-2.3949887683

O,0,2.8055590313,0.3290931946,-2.4907774755

C,0,2.8735089101,0.8662156656,-3.7581064081

C,0,3.5767088903,2.1038383569,-3.7234236662

N,0,3.8033493162,2.8751101419,-4.8620823723

C,0,4.6479561761,4.0475495586,-4.5570456062

O,0,2.3647409063,0.3044500071,-4.7315973275

C,0,4.3357863934,2.1398937755,-6.0360403834

C,0,2.1899713945,3.6792621873,-5.6084659827

C,0,1.5161777438,4.3001082119,-4.5110203628

C,0,0.8224150887,3.5946490011,-3.5861107169

H,0,2.0854127953,-1.1589960154,-1.3396295487

H,0,1.0273973765,-0.7348254806,-2.7220826024

H,0,2.5043873474,-1.6709008558,-3.0045546317

H,0,3.7723845074,2.5764315677,-2.7745382116

H,0,5.3565996967,1.8135453254,-5.815298802

H,0,3.7015356856,1.2731450533,-6.2079763226

H,0,4.3364364197,2.7999139331,-6.9063937099

H,0,5.6271890004,3.7081298844,-4.2057370523

H,0,4.7661422239,4.6547759786,-5.4561324921

H,0,4.1643840525,4.6379703543,-3.7788518199

H,0,2.5792527864,4.3181698051,-6.3983353189

H,0,1.7814100718,2.7378480939,-5.9632579432

H,0,1.694026347,5.361589017,-4.338810724

H,0,0.6013579429,2.5414882109,-3.7259886299

H,0,0.4133513358,4.0690018654,-2.6967931205

Cation- M11/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMM11gasSB

parent sm conf 2

M11/6-31G*

E(RM11) = -519.142571310

Zero-point correction= 0.241770 (Hartree/Particle)

Thermal correction to Energy= 0.254466

Thermal correction to Enthalpy= 0.255410

Thermal correction to Gibbs Free Energy= 0.202889

Sum of electronic and ZPE= -518.900801

Sum of electronic and thermal Energies= -518.888106

Sum of electronic and thermal Enthalpies= -518.887161

Sum of electronic and thermal Free Energies= -518.939682

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.680	46.631	110.538

C,0,1.9777653427,-0.724564256,-2.2697283594

O,0,2.7644748543,0.4849157165,-2.4058020397

C,0,2.7800558254,1.0284344229,-3.605373081

O,0,2.197323612,0.6111407864,-4.5793859447

C,0,3.6508301703,2.2821720087,-3.5753892338

N,0,3.7392644197,2.9936208194,-4.8916761776

C,0,4.4491430357,2.1453357192,-5.9059859817

C,0,4.5291515871,4.2471006541,-4.6630192358

C,0,2.3607710458,3.3775792004,-5.4519117832

C,0,1.4575323012,3.9676195651,-4.4086456984

C,0,1.2091478735,5.272964765,-4.3272031703

H,0,2.0783060943,-1.021131132,-1.2236455195

H,0,0.9333567333,-0.5116267349,-2.523845206

H,0,2.3739510009,-1.4945506306,-2.941054651

H,0,4.6692052301,2.0075247347,-3.2685419395

H,0,3.2485765464,2.9820484049,-2.8314000884

H,0,3.8873447831,1.2167699119,-6.0414061679

H,0,4.4939226244,2.7045790366,-6.8477003666

H,0,5.4647629868,1.9408712053,-5.5463292408

H,0,5.4964933939,3.985257209,-4.2186481311

H,0,4.6853506927,4.742387762,-5.6282338547

H,0,3.9621839132,4.9001229133,-3.9898238223

H,0,2.5703126184,4.0955819709,-6.2558762662

H,0,1.9396877488,2.4610612708,-5.8759580559

H,0,0.9457579364,3.2665942988,-3.7431522247

H,0,1.6702062376,5.9896337601,-5.0128104685

H,0,0.5141533917,5.6758746174,-3.5897762916

TS- M11/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSM11gasSB

parent ts exo s-cis

M11/6-31G*

E(RM11) = -518.681738827

Zero-point correction= 0.225643 (Hartree/Particle)

Thermal correction to Energy= 0.237656

Thermal correction to Enthalpy= 0.238600

Thermal correction to Gibbs Free Energy= 0.188571

Sum of electronic and ZPE= -518.456096

Sum of electronic and thermal Energies= -518.444083

Sum of electronic and thermal Enthalpies= -518.443139

Sum of electronic and thermal Free Energies= -518.493167

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.131	45.275	105.293

C,0,1.9891134653,-0.8093901821,-2.4488932146

O,0,2.7070229288,0.4200475128,-2.4866945061

C,0,2.765405726,0.9995430201,-3.7156832699

C,0,3.3875988892,2.2833395402,-3.6771745216

N,0,3.7481725741,2.921696739,-4.864553138

C,0,4.5868813635,4.0965560758,-4.5906438888

O,0,2.2461124317,0.4672150204,-4.6972788123

C,0,4.311828711,2.1035493414,-5.9559156176

C,0,2.1518926684,3.6950105842,-5.6691014682

C,0,1.5487853978,4.2469954885,-4.5225144534

C,0,1.1950642762,3.3349593906,-3.5594354206

H,0,2.0138825675,-1.1425089673,-1.4060518138

H,0,0.9523946859,-0.6648980083,-2.781793654

H,0,2.4611112764,-1.5551415419,-3.1022938667

H,0,3.8010437438,2.6572188581,-2.7468082112

H,0,5.3318486052,1.7874184157,-5.6924014585

H,0,3.6723294771,1.2300130511,-6.1046590573

H,0,4.3407826217,2.7152588416,-6.8685939124

H,0,5.5400617114,3.7785560409,-4.1429106453

H,0,4.7777456351,4.6354044452,-5.5273922923

H,0,4.0502124445,4.7488890899,-3.891114336

H,0,2.5444667778,4.340470511,-6.4621241519

H,0,1.7790684728,2.7240293595,-6.0137324483

H,0,1.7225607029,5.2942802939,-4.2640794072

H,0,0.8393544739,2.3490592398,-3.8625225706

H,0,0.9495123722,3.6398888401,-2.5396738631

Cation- SOGGA11X/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMSOGGA11XgasSB

parent sm conf 2

SOGGA11X/6-31G*

E(RSOGGA11X) = -519.282912340

Zero-point correction= 0.246556 (Hartree/Particle)

Thermal correction to Energy= 0.259214

Thermal correction to Enthalpy= 0.260159

Thermal correction to Gibbs Free Energy= 0.207596

Sum of electronic and ZPE= -519.036356

Sum of electronic and thermal Energies= -519.023698

Sum of electronic and thermal Enthalpies= -519.022754

Sum of electronic and thermal Free Energies= -519.075316

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.660	46.153	110.628

C,0,2.0346290851,-0.8052187547,-2.2744266965

O,0,2.7798372036,0.4271214551,-2.4180481469

C,0,2.783383088,0.9695801425,-3.6180540196

O,0,2.2211340968,0.5441651978,-4.598339211

C,0,3.6267510831,2.2415403963,-3.5671917205

N,0,3.7201950627,2.9909512364,-4.8641618568

C,0,4.4145260975,2.161008048,-5.9049953949

C,0,4.5351958172,4.2223575564,-4.6089408928

C,0,2.3413290031,3.4024544034,-5.4074555797

C,0,1.4761337744,4.0946492165,-4.4000964787

C,0,1.192153366,5.3967875287,-4.4575718715

H,0,2.1563386387,-1.0862445989,-1.2309185839

H,0,0.985214809,-0.6313809143,-2.5149498917

H,0,2.4496266477,-1.565370226,-2.937246478

H,0,4.6434020769,1.9816957645,-3.2589329609

H,0,3.2155630252,2.9167622552,-2.8132524146

H,0,3.8334823429,1.2575235556,-6.0793081771

H,0,4.4870539979,2.749960652,-6.8204886154

H,0,5.4156608138,1.9143374003,-5.5462133974

H,0,5.5049290463,3.9302699871,-4.2027160911

H,0,4.6753517609,4.7487851157,-5.5542433955

H,0,4.0033993626,4.8607273357,-3.9031335815

H,0,2.5564218572,4.0512096541,-6.2603115065

H,0,1.8810957098,2.479219093,-5.760363031

H,0,0.9990250355,3.472014199,-3.645143831

H,0,1.6078749826,6.0455647463,-5.2256769479

H,0,0.509324215,5.8568475542,-3.7501422279

TS- SOGGA11X/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSSOGGA11XgasSB

parent ts exo s-cis

SOGGA11X/6-31G*

E(RSOGGA11X) = -518.818183233

Zero-point correction= 0.229415 (Hartree/Particle)

Thermal correction to Energy= 0.241663

Thermal correction to Enthalpy= 0.242607

Thermal correction to Gibbs Free Energy= 0.191836

Sum of electronic and ZPE= -518.588768

Sum of electronic and thermal Energies= -518.576520

Sum of electronic and thermal Enthalpies= -518.575576

Sum of electronic and thermal Free Energies= -518.626347

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.646	45.392	106.857

C,0,2.0337956752,-0.8187408272,-2.3949807224

O,0,2.7180805973,0.4236866169,-2.4739637608

C,0,2.773443403,0.9659157892,-3.7215106847

C,0,3.4063919793,2.2454924329,-3.6981029262

N,0,3.7645657372,2.9103700611,-4.8651545267

C,0,4.6379809469,4.0537689972,-4.5789114214

O,0,2.2807844988,0.3956795036,-4.69325368

C,0,4.2907408998,2.1019757374,-5.9793170045

C,0,2.1477188206,3.7859572252,-5.686533522

C,0,1.5265065228,4.2673873471,-4.5177777758

C,0,1.076673442,3.3466883371,-3.6097101842

H,0,2.0716764058,-1.1070857628,-1.3432247689

H,0,0.9950507205,-0.7198215734,-2.7225121952

H,0,2.5220269049,-1.5773289759,-3.0129346484

H,0,3.7415074933,2.6610344708,-2.7596500419

H,0,5.2991249677,1.7477658166,-5.7356020282

H,0,3.6299508578,1.2523574658,-6.1390331721

H,0,4.3310371666,2.7278634638,-6.8757105221

H,0,5.582805209,3.707154576,-4.1444599574

H,0,4.8388529528,4.5991286422,-5.5039700156

H,0,4.1337230432,4.7147805558,-3.8708055681

H,0,2.5638686248,4.4797492496,-6.4155815945

H,0,1.790135353,2.8466999687,-6.1026417233

H,0,1.6984491657,5.297389436,-4.2085335832

H,0,0.7771653502,2.3568544215,-3.9368977865

H,0,0.7821972621,3.6327380251,-2.6032661855

Cation- M11L/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMM11LgasSB

parent sm conf 2

M11L/6-31G*

E(RM11L) = -519.255175775

Zero-point correction= 0.235966 (Hartree/Particle)

Thermal correction to Energy= 0.249184

Thermal correction to Enthalpy= 0.250128

Thermal correction to Gibbs Free Energy= 0.195337

Sum of electronic and ZPE= -519.019210

Sum of electronic and thermal Energies= -519.005991

Sum of electronic and thermal Enthalpies= -519.005047

Sum of electronic and thermal Free Energies= -519.059839

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	156.366	47.624	115.319

C,0,2.0249147956,-0.7192511392,-2.300208613

O,0,2.7830186235,0.4827623455,-2.4221330613

C,0,2.7835477207,1.007634739,-3.6116546375

O,0,2.2161253562,0.5894905091,-4.5754859232

C,0,3.633177064,2.2599182229,-3.5752519294

N,0,3.7207070389,2.979459038,-4.867257703

C,0,4.4075019531,2.1567610104,-5.8852386471

C,0,4.5172082092,4.1998834618,-4.6280670379

C,0,2.3595395452,3.3816085125,-5.409560424

C,0,1.4822239535,4.0181077826,-4.3996037916

C,0,1.2051102439,5.315454341,-4.3986103643

H,0,2.149706884,-1.0318233023,-1.2590035086

H,0,0.9676862451,-0.5224064929,-2.5265731952

H,0,2.4139315682,-1.4821342216,-2.9884588403

H,0,4.6592027506,2.0032521956,-3.2630047457

H,0,3.2370436649,2.958675112,-2.820321011

H,0,3.8348381228,1.2382766831,-6.0603969479

H,0,4.4735419438,2.7384503028,-6.8150093297

H,0,5.4211089847,1.9193348446,-5.5325203503

H,0,5.4949821761,3.920236815,-4.2117441472

H,0,4.6621624918,4.724563835,-5.5825479297

H,0,3.9810527841,4.8510339901,-3.9237934385

H,0,2.5817914243,4.0686418923,-6.2439053264

H,0,1.9157819206,2.4613828366,-5.8176175697

H,0,0.9770031942,3.3536359843,-3.6853427584

H,0,1.6444746864,6.0014659965,-5.1339984131

H,0,0.5016486542,5.7529027051,-3.6850133562

TS- M11L/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSM11LgasSB

parent ts exo s-cis

M11L/6-31G*

E(RM11L) = -518.813902185

Zero-point correction= 0.219337 (Hartree/Particle)

Thermal correction to Energy= 0.232165

Thermal correction to Enthalpy= 0.233109

Thermal correction to Gibbs Free Energy= 0.181072

Sum of electronic and ZPE= -518.594565

Sum of electronic and thermal Energies= -518.581737

Sum of electronic and thermal Enthalpies= -518.580793

Sum of electronic and thermal Free Energies= -518.632830

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 145.686 47.472 109.521

C,0,2.0005719324,-0.7485365973,-2.4426445577

O,0,2.742958879,0.4319150475,-2.4901268005

C,0,2.8420877931,0.9494421424,-3.7263555714

C,0,3.5623865725,2.1730797313,-3.6975902581

N,0,3.8367406597,2.8657306597,-4.8363407126

C,0,4.6381675029,4.0372883549,-4.5802791724

O,0,2.349549803,0.4014241047,-4.6902734874

C,0,4.3260254718,2.1167975711,-5.9766336208

C,0,2.1139310834,3.7163874351,-5.6644085453

C,0,1.5289998968,4.2110635575,-4.492862903

C,0,1.0094709782,3.3697748706,-3.5658674332

H,0,2.0094864201,-1.0665215251,-1.3909913357

H,0,0.961693272,-0.5878204298,-2.7783806163

H,0,2.4439086491,-1.533643631,-3.0775203529

H,0,3.7560864057,2.6690506336,-2.7483698432

H,0,5.3564892449,1.7668468572,-5.7809278421

H,0,3.6737773083,1.2537186896,-6.1533665782

H,0,4.3272495644,2.7761072388,-6.8591994662

H,0,5.632658852,3.7493229201,-4.1921300074

H,0,4.7626493405,4.6129316609,-5.5094675658

H,0,4.1302671163,4.6651300519,-3.8323630904

H,0,2.4955567164,4.4040818315,-6.4302352538

H,0,1.7758408228,2.7414356712,-6.0383592099

H,0,1.698354791,5.264529982,-4.2255532245

H,0,0.7545099446,2.3389365408,-3.8330279672

H,0,0.6848349794,3.718987631,-2.5807645839

Cation- MN12L/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMMN12LgasSB

parent sm conf 2

MN12L/6-31G*

E(RMN12L) = -518.878893022

Zero-point correction= 0.243781 (Hartree/Particle)

Thermal correction to Energy= 0.256324

Thermal correction to Enthalpy= 0.257269

Thermal correction to Gibbs Free Energy= 0.205211

Sum of electronic and ZPE= -518.635112

Sum of electronic and thermal Energies= -518.622569

Sum of electronic and thermal Enthalpies= -518.621624

Sum of electronic and thermal Free Energies= -518.673682

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 160.846 46.202 109.565

C,0,1.982134696,-0.6898426066,-2.2606374093

O,0,2.7814197438,0.4950011646,-2.4133649704

C,0,2.7647421192,1.0483673982,-3.6011724494

O,0,2.1457677112,0.6593302107,-4.5600651829

C,0,3.6466517985,2.2822574125,-3.5814425652

N,0,3.7410069395,2.9866473258,-4.8983366183

C,0,4.450049639,2.1414510338,-5.906332346

C,0,4.5349044362,4.2302470095,-4.6641876294

C,0,2.3708407484,3.3916277727,-5.4734184211

C,0,1.4488009829,3.9285191179,-4.4317097179

C,0,1.1950508761,5.2283637095,-4.2949113784

H,0,2.1124466052,-0.9940357112,-1.2236706304

H,0,0.9353355799,-0.4602190776,-2.4750099681

H,0,2.3356979391,-1.4645650755,-2.9455666334

H,0,4.6644488956,2.009725848,-3.2756374682

H,0,3.2618861105,2.9964354257,-2.8426727816

H,0,3.8919387791,1.2146987444,-6.050977395

H,0,4.4992227879,2.7007813353,-6.8451846103

H,0,5.4627214551,1.9358506377,-5.5463732593

H,0,5.4897009942,3.9648963616,-4.2009996046

H,0,4.7131680133,4.7186255415,-5.6262298907

H,0,3.9636290097,4.8915369341,-4.0051979295

H,0,2.6056230976,4.1445481356,-6.2362826087

H,0,1.9691149074,2.4962628402,-5.9542118535

H,0,0.930323994,3.1936420422,-3.8122501762

H,0,1.6660377387,5.9748886034,-4.936758713

H,0,0.4863664016,5.6022758659,-3.5597207896

TS- MN12L/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSMN12LgasSB

parent ts exo s-cis

MN12L/6-31G*

E(RMN12L) = -518.430596673

Zero-point correction= 0.225642 (Hartree/Particle)

Thermal correction to Energy= 0.238139

Thermal correction to Enthalpy= 0.239083

Thermal correction to Gibbs Free Energy= 0.187929

Sum of electronic and ZPE= -518.204955

Sum of electronic and thermal Energies= -518.192458

Sum of electronic and thermal Enthalpies= -518.191514

Sum of electronic and thermal Free Energies= -518.242668

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.434	46.378	107.663

C,0,1.9478226148,-0.7680069572,-2.4484615478

O,0,2.7271891489,0.407736052,-2.4937929803

C,0,2.8308958241,0.9656074106,-3.7228223348

C,0,3.569497527,2.1782221256,-3.6837587388

N,0,3.8579146469,2.869804375,-4.8375990226

C,0,4.6241725409,4.0819853814,-4.5822755942

O,0,2.3019736506,0.4555964719,-4.7071366689

C,0,4.3643466891,2.1245989844,-5.9917725842

C,0,2.078862244,3.6752397134,-5.6749358345

C,0,1.5331491583,4.2027144903,-4.4981659585

C,0,1.0627783473,3.3637568485,-3.5299113797

H,0,1.9563689,-1.0925457019,-1.4058044224

H,0,0.9196199243,-0.5744343671,-2.7769294217

H,0,2.3699774433,-1.54722473,-3.0933971624

H,0,3.8265330922,2.6396618578,-2.7378888254

H,0,5.3998473641,1.8048350325,-5.8036405319

H,0,3.7319322879,1.2521431756,-6.1627031884

H,0,4.3414215554,2.7843177103,-6.8674562051

H,0,5.621556246,3.8322755214,-4.1905390956

H,0,4.7284219047,4.6501346646,-5.5123900345

H,0,4.0870533912,4.6869934679,-3.8436719635

H,0,2.4710371565,4.3216841523,-6.460995412

H,0,1.7839012825,2.6706754247,-5.982544383

H,0,1.6949138813,5.2582295,-4.2675626212

H,0,0.8060203073,2.3352026433,-3.7761457009

H,0,0.7770468718,3.7182577527,-2.5417383875

Cation- N12/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMN12gasSB

parent sm conf 2

N12/6-31G*

E(RN12) = -519.298176840

Zero-point correction= 0.241070 (Hartree/Particle)

Thermal correction to Energy= 0.253204

Thermal correction to Enthalpy= 0.254148

Thermal correction to Gibbs Free Energy= 0.202914

Sum of electronic and ZPE= -519.057107

Sum of electronic and thermal Energies= -519.044973

Sum of electronic and thermal Enthalpies= -519.044028

Sum of electronic and thermal Free Energies= -519.095263

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.888	45.268	107.831

C,0,2.059856015,-0.8262562526,-2.2923624338

O,0,2.7934728317,0.4010963822,-2.4373966514

C,0,2.7878456781,0.9628714489,-3.6246860965

O,0,2.2228646096,0.5465605028,-4.6079118481

C,0,3.6166863846,2.237734902,-3.5589343712

N,0,3.7163160055,2.9898559463,-4.8493959032

C,0,4.4008880016,2.1611747867,-5.8894396309

C,0,4.5267611147,4.2166820338,-4.5940611027

C,0,2.3312228264,3.4022100176,-5.3849391727

C,0,1.4932104758,4.1321874268,-4.3989768129

C,0,1.2010091727,5.4283504441,-4.5048925767

H,0,2.2277134011,-1.1415052139,-1.2706231515

H,0,1.0046247544,-0.6462022764,-2.4748394882

H,0,2.4334735551,-1.5645816117,-2.9952394849

H,0,4.6276816917,1.9936291123,-3.2406005433

H,0,3.1941282197,2.90769644,-2.8149807181

H,0,3.8122473911,1.2693091357,-6.0619881038

H,0,4.4776977498,2.7488796157,-6.7979912786

H,0,5.3936180237,1.9050989379,-5.5324763091

H,0,5.4880065936,3.9287702755,-4.1810274254

H,0,4.6721701779,4.7370413664,-5.5349528914

H,0,3.9894591887,4.853587062,-3.900257469

H,0,2.5439041612,4.0106944055,-6.2597477656

H,0,1.8678519889,2.4701198896,-5.6929422745

H,0,1.0380318972,3.5457460782,-3.610771825

H,0,1.5936270266,6.0433267043,-5.3041579261

H,0,0.5346630633,5.9132404402,-3.8067297458

TS- N12/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSN12gasSB

parent ts exo s-cis

N12/6-31G*

E(RN12) = -518.850311079

Zero-point correction= 0.223991 (Hartree/Particle)

Thermal correction to Energy= 0.236726

Thermal correction to Enthalpy= 0.237670

Thermal correction to Gibbs Free Energy= 0.185716

Sum of electronic and ZPE= -518.626320

Sum of electronic and thermal Energies= -518.613585

Sum of electronic and thermal Enthalpies= -518.612641

Sum of electronic and thermal Free Energies= -518.664596

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.548	46.890	109.348

C,0,2.0432916881,-0.8451035306,-2.4454135796

O,0,2.7402871057,0.3787150029,-2.4998686936

C,0,2.8189259179,0.9465613132,-3.7346546297

C,0,3.5146914936,2.1789017487,-3.693552363

N,0,3.7927970122,2.8903745549,-4.8492593075

C,0,4.62799759,4.0589385695,-4.5724749815

O,0,2.3120175886,0.4102621972,-4.7207350884

C,0,4.314306732,2.110305683,-5.9810457707

C,0,2.1651498674,3.6863875275,-5.6392528991

C,0,1.5341870422,4.2777095948,-4.5207485308

C,0,0.9708551756,3.4985970545,-3.5631162237

H,0,2.0634967121,-1.1539618195,-1.4044854617

H,0,1.0132621228,-0.7328769916,-2.7819753982

H,0,2.5210454435,-1.600325607,-3.0687922825

H,0,3.771408036,2.6328425939,-2.7551804899

H,0,5.3295602305,1.784347169,-5.7575373483

H,0,3.6718846435,1.2484563379,-6.1196997601

H,0,4.31719364,2.7346765504,-6.8711639953

H,0,5.5866011554,3.7393237887,-4.1652822987

H,0,4.7862602532,4.617719147,-5.4900439568

H,0,4.1180661133,4.6877361163,-3.8490770482

H,0,2.5524482335,4.3176097252,-6.4294464613

H,0,1.7909162015,2.7267941379,-5.9699187188

H,0,1.691256693,5.3327431922,-4.3289346834

H,0,0.7405085037,2.4629882055,-3.758415575

H,0,0.6258388048,3.9077387386,-2.6239644539

Cation- N12SX/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMN12SXgasSB

parent sm conf 2

N12SX/6-31G*

E(RN12SX) = -519.152815042

Zero-point correction= 0.245562 (Hartree/Particle)

Thermal correction to Energy= 0.258294

Thermal correction to Enthalpy= 0.259239

Thermal correction to Gibbs Free Energy= 0.206509

Sum of electronic and ZPE= -518.907253

Sum of electronic and thermal Energies= -518.894521

Sum of electronic and thermal Enthalpies= -518.893576

Sum of electronic and thermal Free Energies= -518.946306

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.082	46.416	110.978

C,0,2.0425604974,-0.8052785082,-2.2769344952

O,0,2.7756716394,0.4215287286,-2.4312262312

C,0,2.7867889466,0.9686901233,-3.6252396823

O,0,2.2304965601,0.5422448947,-4.607373687

C,0,3.6227705187,2.2370744476,-3.570254777

N,0,3.7177972538,2.9897075073,-4.8600894305

C,0,4.40835375,2.1665991074,-5.9020847652

C,0,4.5279014626,4.2180131072,-4.6020443805

C,0,2.3393573086,3.4011882712,-5.3973045127

C,0,1.4872588232,4.1049764716,-4.3983032405

C,0,1.2002367547,5.4022303214,-4.4710387085

H,0,2.1613041348,-1.0846822231,-1.2370119741

H,0,0.9956035607,-0.6422729071,-2.5182322305

H,0,2.4560408762,-1.56638468,-2.9331678538

H,0,4.6346304492,1.981224154,-3.2594474605

H,0,3.2103243184,2.9061452076,-2.8182950918

H,0,3.8291485205,1.2680233026,-6.0788892505

H,0,4.4807012595,2.7553160812,-6.812034935

H,0,5.4052762064,1.9173118696,-5.5478944

H,0,5.4931443033,3.9297025897,-4.1950692804

H,0,4.6695446023,4.7446828933,-5.5415127561

H,0,3.9949234873,4.8527932209,-3.9010584775

H,0,2.5499158722,4.0347556145,-6.2563532469

H,0,1.8763257664,2.4785210209,-5.7346305655

H,0,1.0227834093,3.4963083365,-3.6309479259

H,0,1.6033546366,6.0387448183,-5.2494766343

H,0,0.5268170816,5.8701542291,-3.7664070069

TS- N12SX/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSN12SXgasSB

parent ts exo s-cis

N12SX/6-31G*

E(RN12SX) = -518.693748885

Zero-point correction= 0.228453 (Hartree/Particle)

Thermal correction to Energy= 0.240818

Thermal correction to Enthalpy= 0.241762

Thermal correction to Gibbs Free Energy= 0.190717

Sum of electronic and ZPE= -518.465296

Sum of electronic and thermal Energies= -518.452931

Sum of electronic and thermal Enthalpies= -518.451987

Sum of electronic and thermal Free Energies= -518.503031

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.116	45.706	107.433

C,0,2.0342013524,-0.8156767844,-2.4030759169

O,0,2.7174901676,0.4176494315,-2.485695148

C,0,2.7817290626,0.9673869813,-3.7258277046

C,0,3.4226632692,2.2342488281,-3.700232991

N,0,3.7703428624,2.9063045649,-4.8614357202

C,0,4.6304689721,4.0549899545,-4.5788061692

O,0,2.2883260217,0.4036060082,-4.7006734088

C,0,4.2890531059,2.106025795,-5.9791414569

C,0,2.1602709532,3.7657018984,-5.6731762803

C,0,1.5370316123,4.2622972939,-4.5153440952

C,0,1.0648295368,3.3666961502,-3.6029522552

H,0,2.0652786412,-1.107598369,-1.3566637341

H,0,1.0003554722,-0.717535903,-2.7335169848

H,0,2.5167739039,-1.5749786129,-3.0179075582

H,0,3.7426376356,2.6542111971,-2.7638257399

H,0,5.2981613676,1.7622881424,-5.7462260915

H,0,3.6363158683,1.2531190473,-6.1262210249

H,0,4.3136991406,2.7250100126,-6.8746084716

H,0,5.575247152,3.7174136863,-4.1497263248

H,0,4.8234486717,4.6015270832,-5.4988817438

H,0,4.1249279567,4.7072851555,-3.8711735794

H,0,2.5733712232,4.4466529114,-6.4087858767

H,0,1.8004055985,2.8270610359,-6.0760828292

H,0,1.7015125101,5.2943907972,-4.2258204037

H,0,0.7835659699,2.369855645,-3.9092442086

H,0,0.7621459725,3.6695290497,-2.6089942825

Cation- MN12SX/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMMN12SXgasSB

parent sm conf 2

MN12SX/6-31G*

E(RMN12SX) = -518.982546949

Zero-point correction= 0.243079 (Hartree/Particle)

Thermal correction to Energy= 0.255846

Thermal correction to Enthalpy= 0.256790

Thermal correction to Gibbs Free Energy= 0.203916

Sum of electronic and ZPE= -518.739468

Sum of electronic and thermal Energies= -518.726701

Sum of electronic and thermal Enthalpies= -518.725757

Sum of electronic and thermal Free Energies= -518.778631

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.546	46.628	111.283

C,0,1.9988732249,-0.7305065565,-2.2600201146

O,0,2.771498644,0.4737052925,-2.4119993288

C,0,2.7743736917,1.0122810745,-3.6105058473

O,0,2.1878656314,0.5981585411,-4.5802953329

C,0,3.6413666086,2.2626871745,-3.5803765591

N,0,3.7338020949,2.9878940953,-4.8871157883

C,0,4.4374836103,2.1533149433,-5.9117573479

C,0,4.5363126396,4.2261305113,-4.6414857312

C,0,2.3612299291,3.3956450148,-5.4452497141

C,0,1.45926989,3.9938279471,-4.4156552435

C,0,1.1904278466,5.2962012901,-4.357553421

H,0,2.1174369565,-1.0189807117,-1.2140955523

H,0,0.9481160247,-0.5306084736,-2.4958878629

H,0,2.386498369,-1.5071144994,-2.9279663095

H,0,4.6603147109,1.9903056714,-3.2735589017

H,0,3.2471302011,2.9588065948,-2.8283981335

H,0,3.8689299849,1.2349743651,-6.080024512

H,0,4.5018640198,2.7317417363,-6.8395905556

H,0,5.4464278925,1.9253735656,-5.5506472645

H,0,5.5036257273,3.9479854786,-4.2094599377

H,0,4.6930088576,4.7390711657,-5.5961678777

H,0,3.9858710098,4.8757423611,-3.9526735908

H,0,2.5860999065,4.1100562309,-6.2481154371

H,0,1.9302749552,2.4879381432,-5.880609699

H,0,0.9532915171,3.2990237591,-3.740045468

H,0,1.6412281477,6.0104645992,-5.0507844263

H,0,0.4864099079,5.7031986853,-3.6322830433

TS- MN12SX/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSMN12SXgasSB

parent ts exo s-cis

MN12SX/6-31G*

E(RMN12SX) = -518.531483626

Zero-point correction= 0.225892 (Hartree/Particle)

Thermal correction to Energy= 0.238352

Thermal correction to Enthalpy= 0.239297

Thermal correction to Gibbs Free Energy= 0.188205

Sum of electronic and ZPE= -518.305591

Sum of electronic and thermal Energies= -518.293131

Sum of electronic and thermal Enthalpies= -518.292187

Sum of electronic and thermal Free Energies= -518.343279

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.568	46.295	107.532

C,0,1.9726834518,-0.7773424101,-2.4245075482

O,0,2.7166557363,0.4221360397,-2.4852083679

C,0,2.8093143302,0.9686307902,-3.7246066717

C,0,3.5056606665,2.2085097573,-3.6936803286

N,0,3.820737446,2.8879819157,-4.8521859064

C,0,4.6306943811,4.0742789889,-4.5860776173

O,0,2.2979154396,0.4295420185,-4.7038338531

C,0,4.3396305043,2.1187458941,-5.9895327473

C,0,2.1058275696,3.7170551612,-5.6771827594

C,0,1.5309037527,4.215593553,-4.4984708419

C,0,1.0751224359,3.338370215,-3.5576454418

H,0,1.9901522475,-1.0878662433,-1.3750583839

H,0,0.9368718247,-0.620709321,-2.7544939029

H,0,2.4199570187,-1.5553362332,-3.0568979214

H,0,3.7937572798,2.6504730858,-2.7473018634

H,0,5.3662885708,1.7856359095,-5.7749942323

H,0,3.6983760993,1.2516593305,-6.1626710079

H,0,4.3466822454,2.7660106268,-6.8757018649

H,0,5.6116490023,3.7843764261,-4.179632822

H,0,4.7733810988,4.6380483254,-5.5149941964

H,0,4.1095964325,4.7038062628,-3.8554842692

H,0,2.4984841628,4.3917525279,-6.4410687205

H,0,1.7812845848,2.7379872308,-6.0374213772

H,0,1.6952030325,5.2624052181,-4.2297838042

H,0,0.7945877496,2.3245715378,-3.8401564277

H,0,0.7928369367,3.6611443929,-2.5554471221

Cation- APFD/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMAPFDgasSB

parent sm conf 2

APFD/6-31G*

E(RAPFD) = -519.013400141

Zero-point correction= 0.242905 (Hartree/Particle)

Thermal correction to Energy= 0.255680

Thermal correction to Enthalpy= 0.256624

Thermal correction to Gibbs Free Energy= 0.203691

Sum of electronic and ZPE= -518.770496

Sum of electronic and thermal Energies= -518.757720

Sum of electronic and thermal Enthalpies= -518.756776

Sum of electronic and thermal Free Energies= -518.809709

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 160.442 46.721 111.407

C,0,2.0028096039,-0.7579125726,-2.2619185322

O,0,2.7603587791,0.4632020043,-2.4162455456

C,0,2.7814091688,0.9845453544,-3.6278764353

O,0,2.2243469114,0.5511981515,-4.6111524054

C,0,3.6394540636,2.2468650025,-3.5829164071

N,0,3.7310386336,2.9917105354,-4.8811400198

C,0,4.4338062747,2.166178101,-5.9144079196

C,0,4.5255772785,4.2326999792,-4.6263395243

C,0,2.3478707997,3.3889209554,-5.4252883833

C,0,1.46762644,4.0318123241,-4.4039247237

C,0,1.209095971,5.3404113688,-4.3911779487

H,0,2.1094193454,-1.0273131388,-1.2133331446

H,0,0.9563104665,-0.5799938579,-2.5165562483

H,0,2.4146420213,-1.5338731464,-2.9098979408

H,0,4.6563985044,1.9808971814,-3.2798347384

H,0,3.2379070529,2.9309169026,-2.8310324275

H,0,3.8745514656,1.2448743635,-6.0672911412

H,0,4.4801146622,2.7402879783,-6.8410143846

H,0,5.4448562406,1.9509435322,-5.5636323562

H,0,5.4880401968,3.9595136035,-4.1908958582

H,0,4.6835576703,4.7469831526,-5.5754653531

H,0,3.9659466567,4.8742082667,-3.9447142233

H,0,2.5573080645,4.063118037,-6.2599547591

H,0,1.9100098486,2.4657368777,-5.806549687

H,0,0.9733685399,3.3714318976,-3.6924462413

H,0,1.6499418317,6.0223583055,-5.1162701516

H,0,0.5232655079,5.7775968403,-3.6710465001

TS- APFD/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSAPFDgasSB

parent ts exo s-cis

APFD/6-31G*

E(RAPFD) = -518.557977027

Zero-point correction= 0.225785 (Hartree/Particle)

Thermal correction to Energy= 0.238257

Thermal correction to Enthalpy= 0.239201

Thermal correction to Gibbs Free Energy= 0.187940

Sum of electronic and ZPE= -518.332192

Sum of electronic and thermal Energies= -518.319720

Sum of electronic and thermal Enthalpies= -518.318776

Sum of electronic and thermal Free Energies= -518.370037

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.508	46.168	107.888

C,0,1.9937289045,-0.8020044167,-2.4291077463

O,0,2.730001606,0.4091235159,-2.490541345

C,0,2.8010410311,0.9681860397,-3.7338620599

C,0,3.483428446,2.2139905361,-3.6963200822

N,0,3.7891938175,2.902452745,-4.8615945172

C,0,4.6247519225,4.0741334529,-4.5835182219

O,0,2.2850676704,0.4367967457,-4.7201842394

C,0,4.3277308793,2.1152582729,-5.9832572318

C,0,2.1416049357,3.707520644,-5.6634083882

C,0,1.5287765357,4.2402313405,-4.5076307153

C,0,1.0672342554,3.3741322208,-3.5600127737

H,0,2.0288149283,-1.1166398442,-1.3845637083

H,0,0.955214864,-0.6528735846,-2.7427419856

H,0,2.4383568592,-1.5700981119,-3.0699169686

H,0,3.7882668961,2.6478031367,-2.7557179326

H,0,5.349508428,1.7972716314,-5.7481842925

H,0,3.6918729659,1.2437924058,-6.1299061051

H,0,4.332997185,2.7387005427,-6.8818152713

H,0,5.5849078712,3.7560638818,-4.1620234374

H,0,4.7942747803,4.629331006,-5.5086115034

H,0,4.1041126913,4.7127929495,-3.8671037246

H,0,2.5281912802,4.3716465983,-6.4355923111

H,0,1.784992369,2.7452624533,-6.0255997171

H,0,1.6851457731,5.2897273208,-4.2580546778

H,0,0.8039093523,2.3559138448,-3.825891861

H,0,0.7711277521,3.7089456728,-2.5688791825

Cation- B3LYPGD2/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMB3LYPGD2gasSB

parent sm conf 2

B3LYP/6-31G*

E(RB3LYP) = -519.469063285

Zero-point correction= 0.241552 (Hartree/Particle)

Thermal correction to Energy= 0.254302

Thermal correction to Enthalpy= 0.255247

Thermal correction to Gibbs Free Energy= 0.202380

Sum of electronic and ZPE= -519.227512

Sum of electronic and thermal Energies= -519.214761

Sum of electronic and thermal Enthalpies= -519.213817

Sum of electronic and thermal Free Energies= -519.266683

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.577	46.829	111.267

C,0,2.0120125523,-0.795658184,-2.2551387652

O,0,2.7660835457,0.4423961786,-2.4085147979

C,0,2.7805059796,0.9723774595,-3.6214478802

O,0,2.2223442461,0.5353866401,-4.6051757308

C,0,3.629536459,2.2451117016,-3.5723325053

N,0,3.7243172827,2.9931565026,-4.8781997381

C,0,4.4355366868,2.164726503,-5.9176363181

C,0,4.5253941253,4.2413702177,-4.6212595586

C,0,2.3334138209,3.3949467721,-5.4314836681

C,0,1.4667659089,4.0598441364,-4.4082461922

C,0,1.2145591692,5.3707201481,-4.4161492273

H,0,2.1250810206,-1.065377556,-1.2058834009

H,0,0.9645973227,-0.6186678448,-2.5111421068

H,0,2.4321578927,-1.5614798409,-2.9115863339

H,0,4.6490988739,1.9911570342,-3.2683822414

H,0,3.2137381728,2.9291006616,-2.8288961489

H,0,3.857168671,1.2584547265,-6.0903821455

H,0,4.5055751575,2.7606471781,-6.8299442196

H,0,5.4349374075,1.929918175,-5.5436037466

H,0,5.493663564,3.9555702056,-4.2048265746

H,0,4.6614570664,4.7590423601,-5.5728805917

H,0,3.9702137735,4.8702982072,-3.9238561587

H,0,2.5529339766,4.0596256108,-6.2710861051

H,0,1.8926135173,2.4667009538,-5.7944006229

H,0,0.9922163053,3.4134335677,-3.67258706

H,0,1.6487203239,6.0300416977,-5.1660294403

H,0,0.5443891776,5.8244747876,-3.6912517215

TS- B3LYPGD2/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSB3LYPGD2gasSB

parent ts exo s-cis

B3LYP/6-31G*

E(RB3LYP) = -519.013995617

Zero-point correction= 0.224309 (Hartree/Particle)

Thermal correction to Energy= 0.236757

Thermal correction to Enthalpy= 0.237702

Thermal correction to Gibbs Free Energy= 0.186590

Sum of electronic and ZPE= -518.789686

Sum of electronic and thermal Energies= -518.777238

Sum of electronic and thermal Enthalpies= -518.776294

Sum of electronic and thermal Free Energies= -518.827405

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.568	46.386	107.573

C,0,1.968310092,-0.8109111111,-2.425166266

O,0,2.7409934651,0.3892709681,-2.4832019702

C,0,2.8217528981,0.9561725669,-3.7296063155

C,0,3.5403315374,2.1853934614,-3.6909183361

N,0,3.8288211149,2.8880237222,-4.8514167211

C,0,4.6343896871,4.0901946489,-4.5844726125

O,0,2.2885725718,0.4354416434,-4.7162031972

C,0,4.3587890581,2.1225294781,-6.0013669114

C,0,2.1130234799,3.6881080094,-5.6684033134

C,0,1.5220204607,4.2300425766,-4.5057667756

C,0,1.0303953882,3.3928050458,-3.5460792146

H,0,2.003336823,-1.1333925891,-1.3814175982

H,0,0.9324967276,-0.62724625,-2.7337884803

H,0,2.3905506298,-1.5820013809,-3.0793384586

H,0,3.8159147133,2.6312645644,-2.7472902076

H,0,5.386304037,1.8049971112,-5.7826725392

H,0,3.7203565928,1.2544957804,-6.1592115806

H,0,4.3485855006,2.7730448915,-6.8816467222

H,0,5.6141279136,3.8009410622,-4.1831313794

H,0,4.7621929051,4.6485066667,-5.5154417384

H,0,4.1021008337,4.7067489124,-3.8559080086

H,0,2.5101548702,4.3413679984,-6.4426476188

H,0,1.7801858552,2.7076315302,-5.9994403179

H,0,1.685951876,5.2820702843,-4.2734467772

H,0,0.785190152,2.3649409519,-3.789143672

H,0,0.729404817,3.7570204567,-2.5669132673

Cation- PBEPBEGD2/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMPBEPBEGD2gasSB

parent sm conf 2

PBEPBE/6-31G*

E(RPBE-PBE) = -518.800218864

Zero-point correction= 0.234765 (Hartree/Particle)

Thermal correction to Energy= 0.247834

Thermal correction to Enthalpy= 0.248779

Thermal correction to Gibbs Free Energy= 0.195258

Sum of electronic and ZPE= -518.565454

Sum of electronic and thermal Energies= -518.552384

Sum of electronic and thermal Enthalpies= -518.551440

Sum of electronic and thermal Free Energies= -518.604961

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	155.518	48.181	112.644

C,0,2.0073738919,-0.8046730628,-2.2613028956

O,0,2.760987967,0.4412790062,-2.3952965637

C,0,2.7887544964,0.9634314176,-3.6231387302

O,0,2.2423855586,0.5098664036,-4.6190996397

C,0,3.6362625114,2.242466652,-3.5675058886

N,0,3.7281321409,2.9931885727,-4.8759949344

C,0,4.4352785081,2.164416207,-5.9202870541

C,0,4.5250466868,4.2462520182,-4.6215634262

C,0,2.3260454423,3.3893468236,-5.4191979557

C,0,1.4721297477,4.0717876803,-4.3961061523

C,0,1.2152475222,5.3908575164,-4.4247729182

H,0,2.1063945331,-1.080900631,-1.2041060605

H,0,0.9549209018,-0.6315676601,-2.5341776958

H,0,2.4423173702,-1.5723970436,-2.9196748633

H,0,4.6656079508,1.9926397206,-3.26087614

H,0,3.2164827748,2.9331956172,-2.8188017728

H,0,3.8548310831,1.2471351737,-6.0837600916

H,0,4.4940248537,2.7606814853,-6.8429197645

H,0,5.4472221215,1.9344615092,-5.5532036288

H,0,5.5011353136,3.9645895391,-4.1991311107

H,0,4.6625823626,4.7658066472,-5.5815290999

H,0,3.9613420345,4.8813424071,-3.9226862016

H,0,2.5380807458,4.0439614349,-6.2801806175

H,0,1.8809954398,2.4442358209,-5.7633404146

H,0,0.9980268613,3.4343365801,-3.6393963604

H,0,1.6421081092,6.0423486239,-5.1973602959

H,0,0.5453150705,5.8592295404,-3.6969127237

TS- PBEPBEGD2/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSPBEPBEGD2gasSB

parent ts exo s-cis

PBEPBE/6-31G*

E(RPBE-PBE) = -518.358258699

Zero-point correction= 0.218331 (Hartree/Particle)

Thermal correction to Energy= 0.231054

Thermal correction to Enthalpy= 0.231999

Thermal correction to Gibbs Free Energy= 0.180342

Sum of electronic and ZPE= -518.139928

Sum of electronic and thermal Energies= -518.127204

Sum of electronic and thermal Enthalpies= -518.126260

Sum of electronic and thermal Free Energies= -518.177917

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	144.989	47.587	108.720

C,0,1.9656135653,-0.8300421215,-2.4518385062

O,0,2.756856815,0.3653123498,-2.4809800332

C,0,2.8360280592,0.9470999469,-3.7344072178

C,0,3.5770563543,2.165946513,-3.6878333077

N,0,3.8168888188,2.895107686,-4.8577710727

C,0,4.6184309905,4.1062358742,-4.5873970733

O,0,2.2869551665,0.4365712247,-4.7316916538

C,0,4.3665863547,2.1276279199,-6.0047584715

C,0,2.1537260072,3.629318623,-5.6359764469

C,0,1.5312642697,4.240530165,-4.5069493337

C,0,1.0076880224,3.455190891,-3.5158379578

H,0,2.0042902035,-1.1826261622,-1.4096642636

H,0,0.9212835331,-0.625981061,-2.7501079854

H,0,2.3734337437,-1.5959894161,-3.1350878524

H,0,3.8253921343,2.6379323855,-2.7393873936

H,0,5.4056158139,1.8319217615,-5.776052695

H,0,3.7360803042,1.2385372945,-6.1452211687

H,0,4.341753624,2.7703378219,-6.9006025241

H,0,5.6050555879,3.8150254095,-4.1851691282

H,0,4.7414729868,4.6725299896,-5.5237474026

H,0,4.0768622306,4.7180702229,-3.8493651884

H,0,2.527728158,4.254253635,-6.457186469

H,0,1.788933156,2.6375721298,-5.9312837613

H,0,1.6809875476,5.3145667151,-4.3333786612

H,0,0.7933816884,2.399265173,-3.7027561778

H,0,0.6748888647,3.8731460291,-2.5595882538

Cation- BLYPGD2/6-31G*/Gas-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMBLYPGD2gasSB

parent sm conf 2

BLYP/6-31G*

E(RB-LYP) = -519.246526000

Zero-point correction= 0.233764 (Hartree/Particle)

Thermal correction to Energy= 0.246919

Thermal correction to Enthalpy= 0.247863

Thermal correction to Gibbs Free Energy= 0.194107

Sum of electronic and ZPE= -519.012762

Sum of electronic and thermal Energies= -518.999607

Sum of electronic and thermal Enthalpies= -518.998663

Sum of electronic and thermal Free Energies= -519.052419

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	154.944	48.505	113.139

C,0,2.0020733179,-0.8342278411,-2.2399661743

O,0,2.7642518002,0.4241074837,-2.3873351283

C,0,2.781192391,0.9542301473,-3.6191664494

O,0,2.2239891854,0.5077753807,-4.6154117603

C,0,3.6358800055,2.2398941888,-3.5612457205

N,0,3.732166468,2.9973940987,-4.8812135516

C,0,4.4484508407,2.1613744333,-5.9334759605

C,0,4.537689949,4.2604126701,-4.6222111149

C,0,2.3163266975,3.4029166335,-5.4383755511

C,0,1.4556417791,4.0799053239,-4.4081271361

C,0,1.2066295076,5.4023766198,-4.4223047193

H,0,2.1143523456,-1.1025611498,-1.1824998333

H,0,0.9492277009,-0.6551338239,-2.5046211844

H,0,2.4332152568,-1.5999431009,-2.9020503237

H,0,4.6644399409,1.9906714225,-3.2576124556

H,0,3.2130919865,2.9318050572,-2.8184836948

H,0,3.8632287764,1.2498763243,-6.1007111865

H,0,4.5133311527,2.7642593631,-6.8502929563

H,0,5.4551494398,1.9282302242,-5.5565099571

H,0,5.5111223927,3.9721984874,-4.2004062992

H,0,4.6730100294,4.777219739,-5.5827925081

H,0,3.9720352653,4.8905240419,-3.9228314938

H,0,2.5412099687,4.064046856,-6.2887897274

H,0,1.8789735008,2.4600941747,-5.7897161882

H,0,0.9836167839,3.4347541866,-3.65905253

H,0,1.6399543994,6.0583356536,-5.1861555425

H,0,0.5387811178,5.8667814051,-3.6909638532

TS- BLYPGD2/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSBLYPGD2gasSB

parent ts exo s-cis

BLYP/6-31G*

E(RB-LYP) = -518.802483883

Zero-point correction= 0.217751 (Hartree/Particle)

Thermal correction to Energy= 0.230467

Thermal correction to Enthalpy= 0.231411

Thermal correction to Gibbs Free Energy= 0.179669

Sum of electronic and ZPE= -518.584733

Sum of electronic and thermal Energies= -518.572017

Sum of electronic and thermal Enthalpies= -518.571073

Sum of electronic and thermal Free Energies= -518.622815

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	144.620	47.562	108.901

C,0,1.9526796919,-0.8589732551,-2.4611378494

O,0,2.7669889982,0.334230627,-2.4850139691

C,0,2.8530930814,0.9381958996,-3.7433024552

C,0,3.6487427001,2.1160139839,-3.6947519963

N,0,3.8050882369,2.9012980677,-4.8753423121

C,0,4.6114762734,4.1273889928,-4.5899498741

O,0,2.2663247113,0.4555567391,-4.742185424

C,0,4.393806834,2.1486312149,-6.0394217975

C,0,2.2047178956,3.5436870819,-5.5775384101

C,0,1.5330923785,4.2399043554,-4.4960265774

C,0,0.9444332011,3.5377702343,-3.4885042566

H,0,1.9931115995,-1.2185237057,-1.4211803794

H,0,0.9103510171,-0.6374822461,-2.7529523497

H,0,2.3477279189,-1.6245128677,-3.1521774969

H,0,3.876080684,2.6051140883,-2.7514354819

H,0,5.4294441001,1.8715464375,-5.7856775497

H,0,3.7778300748,1.2538154634,-6.1920859799

H,0,4.3721686366,2.8028856662,-6.9266314472

H,0,5.6038255981,3.8233865008,-4.2189984477

H,0,4.7060737671,4.7140695379,-5.5162516485

H,0,4.0806993149,4.7100247171,-3.8233231656

H,0,2.5389764639,4.1358999744,-6.4389646446

H,0,1.7976695041,2.5599865041,-5.8368379737

H,0,1.6608799668,5.3260134762,-4.4101658887

H,0,0.7916861932,2.4601469888,-3.5787179168

H,0,0.5472851585,4.0313865234,-2.5954647077

Cation- BP86GD2/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMBP86GD2gasSB

parent sm conf 2

BP86/6-31G*

E(RB-P86) = -519.455853943

Zero-point correction= 0.233913 (Hartree/Particle)

Thermal correction to Energy= 0.246996

Thermal correction to Enthalpy= 0.247940

Thermal correction to Gibbs Free Energy= 0.194389

Sum of electronic and ZPE= -519.221941

Sum of electronic and thermal Energies= -519.208858

Sum of electronic and thermal Enthalpies= -519.207914

Sum of electronic and thermal Free Energies= -519.261465

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	154.992	48.284	112.707

C,0,2.0052877382,-0.8108729891,-2.2580323634

O,0,2.759767265,0.4408860792,-2.3929050776

C,0,2.7870508145,0.9632755588,-3.6224776026

O,0,2.2410504503,0.5086667685,-4.6196073905

C,0,3.6342563584,2.2454910787,-3.5658547032

N,0,3.7268865988,2.9940615434,-4.8784479222

C,0,4.4387653046,2.1630784333,-5.9218692857

C,0,4.5221022187,4.2518850204,-4.6248239011

C,0,2.3221599071,3.3877557774,-5.4256407806

C,0,1.4692484632,4.0687145083,-4.3975007103

C,0,1.2239396362,5.3912811836,-4.4183606513

H,0,2.1027522685,-1.0828806386,-1.1985684166

H,0,0.9532480359,-0.6376842882,-2.5361737032

H,0,2.4464032973,-1.5776627219,-2.9149821863

H,0,4.6648125326,1.9984366321,-3.2583338232

H,0,3.2095894448,2.9388175666,-2.8211149649

H,0,3.8565446359,1.2458606874,-6.0852377038

H,0,4.4991934272,2.7614895771,-6.8442786698

H,0,5.4499369284,1.9343185557,-5.5487895232

H,0,5.4987608129,3.9706382273,-4.2006819172

H,0,4.6576204356,4.7687387546,-5.5876769622

H,0,3.9531200682,4.8851282919,-3.9269586044

H,0,2.5363376489,4.0449890449,-6.2852561675

H,0,1.8803409234,2.4404389789,-5.7695884901

H,0,0.9941116707,3.4284894593,-3.6429946664

H,0,1.6567739433,6.0416417252,-5.1899138871

H,0,0.5589711713,5.862335185,-3.6862529259

TS- BP86GD2/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSBP86GD2gasSB

parent ts exo s-cis

BP86/6-31G*

E(RB-P86) = -519.013386628

Zero-point correction= 0.217497 (Hartree/Particle)

Thermal correction to Energy= 0.230215

Thermal correction to Enthalpy= 0.231159

Thermal correction to Gibbs Free Energy= 0.179558

Sum of electronic and ZPE= -518.795890

Sum of electronic and thermal Energies= -518.783172

Sum of electronic and thermal Enthalpies= -518.782227

Sum of electronic and thermal Free Energies= -518.833828

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 144.462 47.673 108.604

C,0,1.954864405,-0.8317341601,-2.4541109656

O,0,2.7560388656,0.3622973541,-2.4800428328

C,0,2.8361995055,0.9493221631,-3.733461069

C,0,3.5858886904,2.1640218513,-3.684856936

N,0,3.8220446112,2.8943605146,-4.8569996344

C,0,4.6159785945,4.1137786549,-4.5886062755

O,0,2.2810020811,0.4455846899,-4.7327653771

C,0,4.3744023315,2.1291577173,-6.0076786406

C,0,2.1471019453,3.6201415957,-5.6375820664

C,0,1.5314486002,4.2375369696,-4.5067923282

C,0,1.0162178615,3.4529020367,-3.5085854761

H,0,1.9879759055,-1.1836728205,-1.4102936503

H,0,0.9129098183,-0.6191119,-2.7581897804

H,0,2.3630354803,-1.5993519578,-3.1370440852

H,0,3.8331343691,2.6378719693,-2.7362335949

H,0,5.4152995229,1.8353494488,-5.7789597345

H,0,3.7432009572,1.239673389,-6.1495128046

H,0,4.3462714373,2.7772049202,-6.9011338441

H,0,5.6057324949,3.8298158077,-4.185325984

H,0,4.7327720414,4.6779830602,-5.5283808731

H,0,4.0664783731,4.7218600583,-3.8515440292

H,0,2.5222725864,4.2394970331,-6.4635662267

H,0,1.7880696945,2.62175879,-5.9202078688

H,0,1.6825421245,5.3130679744,-4.3382709419

H,0,0.8037976263,2.395676698,-3.6941304596

H,0,0.6895740767,3.8724691426,-2.5497645207

Cation- B3LYPGD3/6-31G*/Gas-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMB3LYPGD3gasSB

parent sm conf 2

B3LYP/6-31G*

E(RB3LYP) = -519.456328353

Zero-point correction= 0.242189 (Hartree/Particle)

Thermal correction to Energy= 0.254978

Thermal correction to Enthalpy= 0.255922

Thermal correction to Gibbs Free Energy= 0.202923

Sum of electronic and ZPE= -519.214139

Sum of electronic and thermal Energies= -519.201351

Sum of electronic and thermal Enthalpies= -519.200406

Sum of electronic and thermal Free Energies= -519.253405

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.001	46.841	111.545

C,0,1.9956002557,-0.7824858409,-2.2507694813

O,0,2.7598802421,0.4486715626,-2.4066987088

C,0,2.7817240827,0.9776737163,-3.6203144884

O,0,2.2214690534,0.544739125,-4.6045627973

C,0,3.6432231698,2.2417888666,-3.5739962916

N,0,3.7372452635,2.9951502333,-4.8814621022

C,0,4.4441603345,2.1617566452,-5.926162202

C,0,4.5434551802,4.2447796764,-4.6247560875

C,0,2.338923547,3.4007123817,-5.432556237

C,0,1.4583823837,4.0489398175,-4.4097933162

C,0,1.1872997804,5.3564216695,-4.4012529242

H,0,2.1049787198,-1.0504588944,-1.2017931393

H,0,0.9495800028,-0.6011593733,-2.5054016295

H,0,2.4078989974,-1.5561582893,-2.9013784132

H,0,4.6589579508,1.971783428,-3.2727231864

H,0,3.2429703496,2.9225050407,-2.820188564

H,0,3.8770490418,1.2472235017,-6.0868884859

H,0,4.4996849036,2.7429269655,-6.847805854

H,0,5.4510190909,1.9357862858,-5.569932307

H,0,5.5087737232,3.9652311322,-4.1997367269

H,0,4.6928574366,4.7625824035,-5.5732653534

H,0,3.9924012616,4.8836300754,-3.9344944919

H,0,2.553412571,4.0712662369,-6.2679473906

H,0,1.9011007292,2.4768813679,-5.8083005325

H,0,0.97746107,3.388602294,-3.6906326486

H,0,1.6176005796,6.0394991754,-5.1309260036

H,0,0.5019222788,5.7890287966,-3.678583637

TS- B3LYPGD3/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSB3LYPGD3gasSB

parent ts exo s-cis

B3LYP/6-31G*

E(RB3LYP) = -519.003002963

Zero-point correction= 0.225100 (Hartree/Particle)

Thermal correction to Energy= 0.237522

Thermal correction to Enthalpy= 0.238467

Thermal correction to Gibbs Free Energy= 0.187365

Sum of electronic and ZPE= -518.777903

Sum of electronic and thermal Energies= -518.765481

Sum of electronic and thermal Enthalpies= -518.764536

Sum of electronic and thermal Free Energies= -518.815638

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.048	46.265	107.553

C,0,1.9734601032,-0.8146708279,-2.4318504227

O,0,2.7518366146,0.3812562479,-2.4883390538

C,0,2.831870372,0.9560898236,-3.7329369335

C,0,3.5638621201,2.1749037102,-3.6937655888

N,0,3.8310529442,2.8920096087,-4.8560740662

C,0,4.6478431771,4.0905662383,-4.5851561224

O,0,2.2889094235,0.4429682352,-4.7194483523

C,0,4.3641262834,2.1210010882,-6.0061707231

C,0,2.1249105065,3.6734867924,-5.6516724745

C,0,1.5095573482,4.2278136493,-4.5003028837

C,0,0.9875756196,3.4165243124,-3.5391365312

H,0,2.0128128183,-1.143150745,-1.3911547655

H,0,0.9358558153,-0.6282449772,-2.7298464793

H,0,2.384812211,-1.5876275607,-3.0893459372

H,0,3.8300305003,2.6239106454,-2.7494434989

H,0,5.390090831,1.8049233491,-5.7856222582

H,0,3.7313871849,1.2494479964,-6.160368252

H,0,4.3562369613,2.7586856615,-6.8945024997

H,0,5.6268730086,3.7942155431,-4.1910989585

H,0,4.7790107593,4.6580355829,-5.5088136798

H,0,4.1300700709,4.7093064578,-3.8497928252

H,0,2.498500898,4.3293171702,-6.4354381846

H,0,1.7821262759,2.6988845269,-5.9877493937

H,0,1.6589366001,5.2861622412,-4.2872404671

H,0,0.7621216305,2.3775069698,-3.7505356307

H,0,0.6603839221,3.8041392606,-2.578234017

Cation- M06GD3/6-31G*/Gas-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMM06GD3gasSB

parent sm conf 2

M06/6-31G*

E(RM06) = -519.081480703

Zero-point correction= 0.240007 (Hartree/Particle)

Thermal correction to Energy= 0.252846

Thermal correction to Enthalpy= 0.253791

Thermal correction to Gibbs Free Energy= 0.200825

Sum of electronic and ZPE= -518.841474

Sum of electronic and thermal Energies= -518.828634

Sum of electronic and thermal Enthalpies= -518.827690

Sum of electronic and thermal Free Energies= -518.880656

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.664	47.167	111.477

C,0,2.0361820788,-0.7854522717,-2.2739412444

O,0,2.7905348192,0.4361442766,-2.4180171651

C,0,2.7780446864,0.9867111562,-3.6146648135

O,0,2.1984037178,0.5718387102,-4.5894133394

C,0,3.6217079359,2.2490073561,-3.5651365728

N,0,3.7182918776,2.9902114165,-4.8654198967

C,0,4.4192373124,2.1553270728,-5.8960687886

C,0,4.5274208366,4.2245459595,-4.615896273

C,0,2.3377224084,3.3999996821,-5.4222829188

C,0,1.4642520902,4.062588633,-4.4163432285

C,0,1.2078786099,5.3691732607,-4.4343866417

H,0,2.1976130711,-1.1071662424,-1.2457631988

H,0,0.9768723782,-0.589709812,-2.4607985926

H,0,2.4031355831,-1.534067122,-2.9811217369

H,0,4.642172494,1.9934343743,-3.2529064013

H,0,3.2135548253,2.9327789175,-2.8115602317

H,0,3.8473258059,1.2395170878,-6.0583847773

H,0,4.4809476475,2.7341835861,-6.8220555557

H,0,5.4268197798,1.9261598029,-5.5355826205

H,0,5.4979660687,3.937873894,-4.2003427193

H,0,4.6714186361,4.7458881703,-5.5667218411

H,0,3.990094186,4.8690695574,-3.9148913293

H,0,2.5662825374,4.0658510402,-6.263623776

H,0,1.8936610379,2.4759486127,-5.8020997163

H,0,0.9652704916,3.4169644511,-3.6909719958

H,0,1.6542685677,6.0320656687,-5.1770404467

H,0,0.5219525162,5.8284307611,-3.7268871786

TS- M06GD3/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSM06GD3gasSB

parent ts exo s-cis

M06/6-31G*

E(RM06) = -518.628058088

Zero-point correction= 0.223114 (Hartree/Particle)

Thermal correction to Energy= 0.235669

Thermal correction to Enthalpy= 0.236613

Thermal correction to Gibbs Free Energy= 0.185271

Sum of electronic and ZPE= -518.404944

Sum of electronic and thermal Energies= -518.392389

Sum of electronic and thermal Enthalpies= -518.391445

Sum of electronic and thermal Free Energies= -518.442787

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.884	46.719	108.058

C,0,1.9680973176,-0.7562911585,-2.3940205037

O,0,2.7174962985,0.4404042769,-2.4762215963

C,0,2.8276949231,0.9549171915,-3.7333229112

C,0,3.491852852,2.2148792881,-3.7043735915

N,0,3.8114920455,2.9000953347,-4.8625959103

C,0,4.6526040606,4.0661389357,-4.592111598

O,0,2.3549411054,0.3797123017,-4.7099201997

C,0,4.3246075128,2.1221826146,-6.0002601979

C,0,2.1181759487,3.7600939161,-5.6714219251

C,0,1.5170923377,4.2087357998,-4.48608746

C,0,1.0619163276,3.290028212,-3.5856106593

H,0,1.991236352,-1.0564327926,-1.3431640282

H,0,0.9308747905,-0.5966953514,-2.7160643061

H,0,2.4016642004,-1.54402016,-3.0212089057

H,0,3.7717356038,2.6590411094,-2.7561032367

H,0,5.3503454323,1.7899970192,-5.7865451435

H,0,3.6801840268,1.2546613037,-6.1530596878

H,0,4.3242754684,2.7604446472,-6.8920388968

H,0,5.6255226306,3.7444140858,-4.1941271785

H,0,4.8043664949,4.6322867595,-5.5174291899

H,0,4.153743541,4.7038530817,-3.8547466618

H,0,2.5143593772,4.4673687305,-6.4021855995

H,0,1.7905604582,2.8044361963,-6.0831934044

H,0,1.6721895444,5.2433596187,-4.1712872794

H,0,0.7942020592,2.2866721368,-3.9105967131

H,0,0.7630232911,3.5671779026,-2.5763432155

Cation- PBE1PBEGD3/6-31G*/Gas- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/gas/SMPBE1PBEGD3gasSB

parent sm conf 2

PBE1PBE/6-31G*

E(RPBE1PBE) = -518.839019773

Zero-point correction= 0.243689 (Hartree/Particle)

Thermal correction to Energy= 0.256408

Thermal correction to Enthalpy= 0.257352

Thermal correction to Gibbs Free Energy= 0.204571

Sum of electronic and ZPE= -518.595331

Sum of electronic and thermal Energies= -518.582612

Sum of electronic and thermal Enthalpies= -518.581668

Sum of electronic and thermal Free Energies= -518.634449

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.898	46.506	111.087

C,0,2.0062944289,-0.7613827417,-2.2724209515

O,0,2.7591869686,0.4618729034,-2.4155711566

C,0,2.7894438218,0.9831321489,-3.6245625071

O,0,2.2424930871,0.5427192163,-4.6082294921

C,0,3.639323947,2.2456140433,-3.5784938179

N,0,3.7285628498,2.9901989474,-4.8751266103

C,0,4.4281817148,2.1649959744,-5.9112409728

C,0,4.5261403328,4.2298446911,-4.6228436781

C,0,2.3453531284,3.3869470817,-5.4142035333

C,0,1.4770421226,4.047370064,-4.3961801678

C,0,1.2030521139,5.3518984096,-4.4102217876

H,0,2.1026128875,-1.0344641632,-1.2235956957

H,0,0.9617243152,-0.5873344071,-2.5376504706

H,0,2.4274868238,-1.5337859324,-2.9187264294

H,0,4.6564794727,1.9808615047,-3.2742411179

H,0,3.2359980144,2.9252831224,-2.8235117834

H,0,3.8612164404,1.2495819795,-6.073614578

H,0,4.4839168003,2.7457682949,-6.8335528545

H,0,5.4361064794,1.9379015315,-5.5578487474

H,0,5.4942067892,3.9532130586,-4.2012690505

H,0,4.6725535,4.7496844659,-5.5712179065

H,0,3.9770369578,4.869109256,-3.9301324301

H,0,2.5501700892,4.0496537771,-6.2594259541

H,0,1.8984949692,2.4610450907,-5.7790840972

H,0,0.9979120617,3.4009069078,-3.6624820982

H,0,1.625837531,6.0213338342,-5.1570135927

H,0,0.5222043521,5.795348941,-3.6898615192

TS- PBE1PBEGD3/6-31G*/Gas

/home/bibaswanbiswas/c8/Parentcalcs/gas/TSPBE1PBEGD3gasSB

parent ts exo s-cis

PBE1PBE/6-31G*

E(RPBE1PBE) = -518.383597958

Zero-point correction= 0.226786 (Hartree/Particle)

Thermal correction to Energy= 0.239069

Thermal correction to Enthalpy= 0.240013

Thermal correction to Gibbs Free Energy= 0.189232

Sum of electronic and ZPE= -518.156812

Sum of electronic and thermal Energies= -518.144529

Sum of electronic and thermal Enthalpies= -518.143585

Sum of electronic and thermal Free Energies= -518.194366

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	150.018	45.789	106.878

C,0,2.0081444154,-0.8045555354,-2.4259872825

O,0,2.727654208,0.4153097902,-2.4851389159

C,0,2.7932890595,0.9704163051,-3.7270980651

C,0,3.4554100645,2.2280760581,-3.6947838153

N,0,3.7778938964,2.9067230744,-4.8612469822

C,0,4.6223056692,4.0712702873,-4.5841781788

O,0,2.2851027154,0.4226301634,-4.7063027994

C,0,4.3118423029,2.1093994506,-5.9768979334

C,0,2.1517551861,3.7245304755,-5.667366125

C,0,1.535305838,4.245536357,-4.5110590487

C,0,1.07490222,3.3666502165,-3.5745718316

H,0,2.0423354662,-1.1184127022,-1.3810333419

H,0,0.9693848366,-0.669632798,-2.7450846799

H,0,2.4657054038,-1.5668427202,-3.0645679535

H,0,3.7700038529,2.6561115044,-2.7546999488

H,0,5.3285150475,1.7780906158,-5.73713261

H,0,3.6653930813,1.2453380117,-6.1248994223

H,0,4.3298034978,2.7305614862,-6.8772786454

H,0,5.5793983516,3.7465819703,-4.1601064015

H,0,4.798489322,4.6232762054,-5.5103099162

H,0,4.1069812561,4.7166421555,-3.8694800175

H,0,2.5464346704,4.3950792987,-6.4297017377

H,0,1.7905774886,2.7688022718,-6.0427776918

H,0,1.7002368577,5.2888513992,-4.2444950745

H,0,0.7951948481,2.3575399549,-3.8590370028

H,0,0.7821944444,3.6894877038,-2.5788045783

Cation1- wB97XD/6-31G*/PCM-Conf1

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM1wB97XDSB

parent sm

wb97xd/6-31G*

E(RwB97XD) = -519.349039668

Zero-point correction= 0.245416 (Hartree/Particle)

Thermal correction to Energy= 0.257894

Thermal correction to Enthalpy= 0.258839

Thermal correction to Gibbs Free Energy= 0.206853

Sum of electronic and ZPE= -519.103624

Sum of electronic and thermal Energies= -519.091145

Sum of electronic and thermal Enthalpies= -519.090201

Sum of electronic and thermal Free Energies= -519.142186

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.831	46.030	109.412

C,0,1.9237085968,-0.7009911841,-2.2712416557

O,0,2.7085673332,0.4952306192,-2.4214923847

C,0,2.8061396053,0.9783279222,-3.6474467082

O,0,2.2917186597,0.495846093,-4.6309260638

C,0,3.6754462451,2.2254345317,-3.6033039181

N,0,3.7611743803,2.990802584,-4.8890243394

C,0,4.4754660646,2.1901266305,-5.9391171667

C,0,4.5565129968,4.2335136101,-4.6159653947

C,0,1.4906611062,4.0036861638,-4.4010772706

C,0,0.4054360219,3.387745163,-3.9368372433

C,0,2.380633248,3.3745411543,-5.4282565373

H,0,1.9827105981,-0.9531009281,-1.2149635608

H,0,0.8907043472,-0.5058868744,-2.5638679446

H,0,2.3401216038,-1.5020365205,-2.8837677637

H,0,4.6904796475,1.9394457793,-3.3181237434

H,0,5.4817143637,1.9674646524,-5.5843323304

H,0,3.919734502,1.2725777742,-6.1177851052

H,0,4.5251112857,2.7897304618,-6.8476511901

H,0,5.5391889023,3.9460949835,-4.2428930723

H,0,4.6594435649,4.7891968827,-5.5473289851

H,0,4.0399267517,4.8382874085,-3.8722122518

H,0,2.5802307889,4.0527080015,-6.2611005226

H,0,1.9425648701,2.4563234284,-5.8148981458

H,0,1.7305965328,5.0112693463,-4.0709339623

H,0,0.133577658,2.3872005751,-4.2645197922

H,0,-0.2532874758,3.8690135637,-3.2211862953

H,0,3.2845808013,2.893099178,-2.8347186519

Cation3/wb97xd /6-31G */PCM-Conf3

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM3wB97XDSB

parent sm

wb97xd/6-31G*

E(RwB97XD) = -519.347492531

Zero-point correction= 0.245361 (Hartree/Particle)

Thermal correction to Energy= 0.257882

Thermal correction to Enthalpy= 0.258826

Thermal correction to Gibbs Free Energy= 0.206739

Sum of electronic and ZPE= -519.102132

Sum of electronic and thermal Energies= -519.089611

Sum of electronic and thermal Enthalpies= -519.088667

Sum of electronic and thermal Free Energies= -519.140753

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.823	46.032	109.625

C,0,1.840545096,-0.6285851552,-2.211902471

O,0,2.7078788401,0.4998145189,-2.4221271907

C,0,2.7821632562,0.9583173153,-3.6596763483

O,0,2.1787776926,0.5110340675,-4.6075668602

C,0,3.7670113997,2.1201761753,-3.674215779

N,0,3.8631137516,2.8680628286,-4.9682628563

C,0,4.4033853687,1.9888745483,-6.0573175161

C,0,2.5220292297,3.4091745521,-5.3724515476

C,0,4.7958656997,4.0667583194,-4.7680706143

C,0,6.1618983327,3.7121023219,-4.265276736

C,0,7.2366810194,3.7155484761,-5.0504435815

H,0,1.9210055669,-0.8570634331,-1.1516621644

H,0,0.8147790508,-0.3636387181,-2.4729061316

H,0,2.1731689801,-1.4741613791,-2.8159011911

H,0,4.7569711118,1.7258106805,-3.4360291158

H,0,3.4884980755,2.8304871614,-2.8929872687

H,0,3.7163150059,1.1590003225,-6.2021855108

H,0,4.4816256,2.5833740767,-6.9674254881

H,0,5.3882044118,1.630558635,-5.7611271974

H,0,2.1237605189,4.003141198,-4.549609873

H,0,2.6573444111,4.0361035134,-6.2532646092

H,0,1.8604395578,2.5769621726,-5.5987274538

H,0,4.84929848,4.5555977974,-5.7423275854

H,0,4.2768913893,4.7308381598,-4.0727492777

H,0,6.2638844803,3.5009066149,-3.203885888

H,0,7.1712724523,3.947067107,-6.1108016402

H,0,8.222796221,3.4944441231,-4.6546011039

Cation4wb97xd /6-31G */PCM-Conf4

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM4wB97XDSB

parent sm

wb97xd/6-31G*

E(RwB97XD) = -519.344298249

Zero-point correction= 0.244933 (Hartree/Particle)

Thermal correction to Energy= 0.257625

Thermal correction to Enthalpy= 0.258569

Thermal correction to Gibbs Free Energy= 0.205721

Sum of electronic and ZPE= -519.099365

Sum of electronic and thermal Energies= -519.086674

Sum of electronic and thermal Enthalpies= -519.085729

Sum of electronic and thermal Free Energies= -519.138577

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 161.662 46.229 111.228

C,0,1.7464201509,-0.8957098538,-2.4876160473

O,0,2.4918759703,0.3340159924,-2.4033943576

C,0,2.7556024597,0.9391587238,-3.5520406776

O,0,2.4093437436,0.5497820682,-4.6396957985

C,0,3.5140627841,2.2560900964,-3.4348913183

N,0,4.2431245201,2.5833843818,-2.162261507

C,0,3.2892665687,2.8529279121,-1.0362258881

C,0,5.1819698861,1.476200684,-1.7808853949

C,0,5.0960457714,3.8337310888,-2.4104450655

C,0,4.324819643,5.0197927501,-2.9018941523

C,0,4.055138571,6.0667325495,-2.125439149

H,0,1.6491917334,-1.2400621535,-1.4608630092

H,0,0.7670148169,-0.70466481,-2.9278538095

H,0,2.2952390408,-1.6199643007,-3.0907278798

H,0,2.7911886859,3.054851687,-3.6153856472

H,0,4.2422838102,2.2705445775,-4.2472879659

H,0,2.6989643096,1.9587507894,-0.8561951498

H,0,3.8723661006,3.1089091584,-0.1519830152

H,0,2.6477470035,3.6880525426,-1.3136514177

H,0,5.8191325627,1.2480260689,-2.6355037804

H,0,5.7886680635,1.8163116549,-0.9423086483

H,0,4.6017969719,0.6028112071,-1.4941030653

H,0,5.5806765364,4.0460626011,-1.4556872039

H,0,5.8600476406,3.5300204934,-3.1299925742

H,0,4.0312969207,5.0275443871,-3.9485544901

H,0,4.3581500591,6.0977193385,-1.0815514889

H,0,3.5295196754,6.933579365,-2.5128564986

CationB971/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM2B971SB

parent sm

b971/6-31G*

E(RB971) = -519.341196575

Zero-point correction= 0.241515 (Hartree/Particle)

Thermal correction to Energy= 0.254421

Thermal correction to Enthalpy= 0.255365

Thermal correction to Gibbs Free Energy= 0.202002

Sum of electronic and ZPE= -519.099682

Sum of electronic and thermal Energies= -519.086775

Sum of electronic and thermal Enthalpies= -519.085831

Sum of electronic and thermal Free Energies= -519.139195

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.652	47.113	112.313

C,0,2.0481997595,-0.8355963614,-2.263900018

O,0,2.7941523524,0.3964101093,-2.4107127832

C,0,2.7795414196,0.9488040728,-3.6188778442

O,0,2.1972678847,0.5085253903,-4.589467928

C,0,3.6206381908,2.2271585476,-3.566717081

N,0,3.7151889278,2.9931654679,-4.8634080951

C,0,4.4192398404,2.1704702681,-5.9165444907

C,0,4.5350860199,4.2306443813,-4.5898832342

C,0,2.3289463272,3.4097902687,-5.4097076538

C,0,1.4700905054,4.1280598209,-4.4079619933

C,0,1.1914761198,5.4339900459,-4.4942711652

H,0,2.1794611951,-1.1247473466,-1.2212529619

H,0,0.9927908593,-0.6614395289,-2.489554239

H,0,2.4537946567,-1.5987344422,-2.933438732

H,0,4.639980205,1.9673565834,-3.2641197353

H,0,3.2095599299,2.89811029,-2.8068888959

H,0,3.8358897258,1.2692818522,-6.1022374931

H,0,4.496524302,2.7722056957,-6.8244701981

H,0,5.4163623942,1.9185666315,-5.548453884

H,0,5.505786144,3.9265564412,-4.1930140109

H,0,4.6656293114,4.770646325,-5.5297645055

H,0,4.0038313797,4.8532405099,-3.8682424628

H,0,2.5453373661,4.0410192992,-6.2757834232

H,0,1.8621936736,2.4808824008,-5.7438456452

H,0,1.0115397452,3.5266982693,-3.6230343663

H,0,1.6077059459,6.0605762007,-5.2821896778

H,0,0.5228178187,5.9156768076,-3.7845804825

TS B971/6-31G */PCM-

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSB971SB

23 parent ts

b971/6-31G*

E(RB971) = -518.822074086

Zero-point correction= 0.223785 (Hartree/Particle)

Thermal correction to Energy= 0.236477

Thermal correction to Enthalpy= 0.237422

Thermal correction to Gibbs Free Energy= 0.185598

Sum of electronic and ZPE= -518.598289

Sum of electronic and thermal Energies= -518.585597

Sum of electronic and thermal Enthalpies= -518.584653

Sum of electronic and thermal Free Energies= -518.636476

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.392	46.819	109.072

C,0,2.0308067342,-0.8195092802,-2.3373156405

O,0,2.7284035646,0.4215035118,-2.4541475247

C,0,2.799840733,0.9354309965,-3.7274355177

C,0,3.4429724765,2.2124303111,-3.7167152171

N,0,3.8000538586,2.8999576265,-4.8688369853

C,0,4.6828773078,4.0494947273,-4.5756156907

O,0,2.3256662866,0.3239756617,-4.6942404749

C,0,4.3015366393,2.1137359438,-6.0205865095

C,0,2.1327231281,3.8383212769,-5.6954797921

C,0,1.5032504573,4.2629573876,-4.5048138132

C,0,0.9908575714,3.3301394466,-3.6385841234

H,0,2.0723122913,-1.0823338952,-1.2772190766

H,0,0.9866177272,-0.7200756311,-2.6567756556

H,0,2.5092531967,-1.6027745859,-2.9363681829

H,0,3.719205138,2.6568519319,-2.7700237615

H,0,5.3098341742,1.7402343265,-5.7982344932

H,0,3.6273370924,1.2758595831,-6.1949825672

H,0,4.338622474,2.7651675025,-6.8990463535

H,0,5.6395459299,3.6930711414,-4.1722593737

H,0,4.8590721652,4.6125430353,-5.495757275

H,0,4.194245945,4.6952561816,-3.8410121573

H,0,2.5684712754,4.5640026709,-6.3809988723

H,0,1.7945428688,2.9118706983,-6.1568439202

H,0,1.6738657159,5.2825170552,-4.1553390285

H,0,0.7202699855,2.3375660041,-3.9891603157

H,0,0.6620692628,3.5992673715,-2.6362476778

CationB972/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM2B972SB

parent sm

b972/6-31G*

E(RB972) = -519.313755427

Zero-point correction= 0.243801 (Hartree/Particle)

Thermal correction to Energy= 0.256659

Thermal correction to Enthalpy= 0.257603

Thermal correction to Gibbs Free Energy= 0.204252

Sum of electronic and ZPE= -519.069955

Sum of electronic and thermal Energies= -519.057096

Sum of electronic and thermal Enthalpies= -519.056152

Sum of electronic and thermal Free Energies= -519.109504

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.056	46.762	112.288

C,0,2.0651958293,-0.8361186311,-2.2650402841

O,0,2.8024293002,0.3922849441,-2.4217434659

C,0,2.7767927358,0.9448394976,-3.6248086606

O,0,2.1899072107,0.50653375,-4.5878753458

C,0,3.6108389211,2.2178141732,-3.5737523304

N,0,3.7077103294,2.98987629,-4.8574913237

C,0,4.4081341543,2.1791104727,-5.9107523228

C,0,4.5271215855,4.216016881,-4.5746124078

C,0,2.3330446636,3.4140049375,-5.3998284107

C,0,1.4822507299,4.1445661142,-4.4114501747

C,0,1.1942486208,5.4419218368,-4.5209559793

H,0,2.2073158606,-1.1219111174,-1.226773732

H,0,1.0102560133,-0.6674601081,-2.4779241348

H,0,2.4645891172,-1.5981833357,-2.9332007961

H,0,4.626051375,1.9582338515,-3.2713952915

H,0,3.2033140535,2.8808593529,-2.8107843238

H,0,3.8225329675,1.2884792832,-6.1157288398

H,0,4.4992579616,2.7885839799,-6.8074603624

H,0,5.3966907745,1.9121309289,-5.5417994633

H,0,5.4967262782,3.9091743647,-4.1881652411

H,0,4.6535394981,4.7667927934,-5.5041378218

H,0,4.004659975,4.8299621815,-3.8452443399

H,0,2.551138876,4.0329658936,-6.2694790626

H,0,1.8568233778,2.4921001316,-5.7278745064

H,0,1.0305563358,3.5591049836,-3.6156550997

H,0,1.6013654551,6.0559564584,-5.3185418951

H,0,0.5265400001,5.9296780919,-3.8198473842

TS B972/6-31G */ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSB972SB

23 parent ts

b972/6-31G*

E(RB972) = -518.792886842

Zero-point correction= 0.226030 (Hartree/Particle)

Thermal correction to Energy= 0.238612

Thermal correction to Enthalpy= 0.239556

Thermal correction to Gibbs Free Energy= 0.187975

Sum of electronic and ZPE= -518.566857

Sum of electronic and thermal Energies= -518.554275

Sum of electronic and thermal Enthalpies= -518.553331

Sum of electronic and thermal Free Energies= -518.604911

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.731	46.437	108.561

C,0,2.0531245275,-0.8163374453,-2.330327741

O,0,2.7280617697,0.4286151403,-2.4587459408

C,0,2.8009378682,0.9303098773,-3.7322155494

C,0,3.432212062,2.2066113043,-3.7261546257

N,0,3.7921655312,2.8952948378,-4.8691799346

C,0,4.6815195245,4.0286144516,-4.5699852242

O,0,2.342107168,0.3057175689,-4.6921930626

C,0,4.2870482675,2.1164629314,-6.0185931503

C,0,2.1410185584,3.8514128437,-5.6906697105

C,0,1.5076205674,4.2697029086,-4.5059099668

C,0,0.9730450606,3.343150142,-3.656188388

H,0,2.0941448915,-1.0656872963,-1.2707341928

H,0,1.0118013143,-0.7393701695,-2.6520958049

H,0,2.5445462201,-1.5974960701,-2.914472787

H,0,3.6952374132,2.6544132652,-2.7812614041

H,0,5.283710975,1.7251013202,-5.7937493325

H,0,3.6062207582,1.2927661779,-6.2085779045

H,0,4.3424560936,2.7717094029,-6.8882504403

H,0,5.6333328521,3.662024604,-4.1748120798

H,0,4.860528935,4.5981195718,-5.4809465174

H,0,4.2055898094,4.6707589586,-3.8299724669

H,0,2.582435606,4.5789085749,-6.3649509579

H,0,1.7958648061,2.938115423,-6.1641078362

H,0,1.6819478687,5.2823755292,-4.1492412784

H,0,0.7008379894,2.3565360356,-4.0113952767

H,0,0.6367375625,3.6096311116,-2.6593084264

Cation B97D/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM2B97DSB

parent sm

b97d/6-31G*

E(RB97D) = -519.163158799

Zero-point correction= 0.236252 (Hartree/Particle)

Thermal correction to Energy= 0.249247

Thermal correction to Enthalpy= 0.250192

Thermal correction to Gibbs Free Energy= 0.196526

Sum of electronic and ZPE= -518.926907

Sum of electronic and thermal Energies= -518.913911

Sum of electronic and thermal Enthalpies= -518.912967

Sum of electronic and thermal Free Energies= -518.966633

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	156.405	47.862	112.949

C,0,2.0226896537,-0.8189659294,-2.232896756

O,0,2.7826617643,0.4187469055,-2.3989550608

C,0,2.7720819106,0.9522320877,-3.6271450243

O,0,2.1890576655,0.4982150426,-4.5986125614

C,0,3.6212722947,2.2298140395,-3.5791068391

N,0,3.7213592309,2.9946477193,-4.8827559862

C,0,4.4420133063,2.1747989724,-5.9334515999

C,0,4.5298426899,4.2448405865,-4.602845122

C,0,2.3277114638,3.4090732118,-5.4432601055

C,0,1.4565817842,4.0809353604,-4.4230819506

C,0,1.2092247484,5.4002012961,-4.4380052937

H,0,2.1558105488,-1.0899046477,-1.1811933283

H,0,0.9657883604,-0.6357788962,-2.4660425637

H,0,2.4285731734,-1.5923332608,-2.8978371229

H,0,4.6452406709,1.9744700848,-3.2788447944

H,0,3.2064907621,2.9137349004,-2.8288807629

H,0,3.8572327409,1.2717922886,-6.1242758062

H,0,4.5214435438,2.7878332387,-6.8379771462

H,0,5.4373935544,1.9291513874,-5.5464613698

H,0,5.5033606803,3.9417602959,-4.2024751081

H,0,4.6515726807,4.7831342334,-5.548624205

H,0,3.9791040324,4.8551473933,-3.8800635634

H,0,2.5593576474,4.0713299593,-6.2859277931

H,0,1.8833156635,2.4785600435,-5.809008981

H,0,0.9845327131,3.4393645034,-3.6751012195

H,0,1.6545753767,6.0547436297,-5.1917924847

H,0,0.5407433385,5.8597735539,-3.7077004514

TS B97D/6-31G */ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSB97DSB

23 parent ts

b97d/6-31G*

E(RB97D) = -518.652802726

Zero-point correction= 0.218558 (Hartree/Particle)

Thermal correction to Energy= 0.231416

Thermal correction to Enthalpy= 0.232361

Thermal correction to Gibbs Free Energy= 0.180264

Sum of electronic and ZPE= -518.434244

Sum of electronic and thermal Energies= -518.421386

Sum of electronic and thermal Enthalpies= -518.420442

Sum of electronic and thermal Free Energies= -518.472538

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	145.216	47.762	109.645

C,0,1.9690473826,-0.8287584544,-2.3837629976

O,0,2.7700282427,0.3621798328,-2.4771141184

C,0,2.8427714347,0.9213842748,-3.7510720594

C,0,3.5882247362,2.1351933919,-3.7165196333

N,0,3.8407480504,2.8841964158,-4.868240979

C,0,4.6528136075,4.0933533276,-4.5759207522

O,0,2.2959764435,0.3796533377,-4.7320560102

C,0,4.3832840242,2.1489071815,-6.045268765

C,0,2.1288423127,3.6796445196,-5.6524473203

C,0,1.5071890389,4.2387651013,-4.4983175173

C,0,0.9347301001,3.4321316129,-3.5525354591

H,0,2.0227493005,-1.1361059781,-1.3313458945

H,0,0.9235478976,-0.6271257605,-2.6673315466

H,0,2.3629046443,-1.6257172402,-3.0339025933

H,0,3.8247909967,2.6018700784,-2.7659589481

H,0,5.4150044652,1.8343634315,-5.8240914932

H,0,3.7496024572,1.2776657011,-6.2296968745

H,0,4.3726223535,2.8253692852,-6.9102192762

H,0,5.6438689499,3.787872144,-4.2065239384

H,0,4.7563040224,4.6809743403,-5.4959781601

H,0,4.1319293395,4.6838080944,-3.8123080672

H,0,2.535669056,4.3351580849,-6.4256242567

H,0,1.7778046422,2.7042808362,-5.9953600201

H,0,1.6752533863,5.2971613267,-4.2757942572

H,0,0.7213379065,2.385807867,-3.7722870295

H,0,0.5872092086,3.8254282475,-2.5943620324

Cation B97D/6-31+G/PCM-Conf2**

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM2B97DSS

parent sm

b97d/6-31+G**

E(RB97D) = -519.197401760

Zero-point correction= 0.235116 (Hartree/Particle)

Thermal correction to Energy= 0.248095

Thermal correction to Enthalpy= 0.249039

Thermal correction to Gibbs Free Energy= 0.195683

Sum of electronic and ZPE= -518.962286

Sum of electronic and thermal Energies= -518.949307

Sum of electronic and thermal Enthalpies= -518.948363

Sum of electronic and thermal Free Energies= -519.001719

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	155.682	48.081	112.297

C,0,2.0076945986,-0.8205454672,-2.2221865418

O,0,2.7631441439,0.4233686939,-2.3949424763

C,0,2.783621811,0.9417091154,-3.6306834428

O,0,2.2265966381,0.4701339888,-4.6107363015

C,0,3.6310018547,2.2184754652,-3.5843181267

N,0,3.7240257258,2.9934231153,-4.882986676

C,0,4.4427615318,2.1856943121,-5.9466955699

C,0,4.5357217272,4.2416542284,-4.5943732799

C,0,2.3299434327,3.4120657582,-5.4351124407

C,0,1.464615024,4.0905381425,-4.4129789521

C,0,1.1899969665,5.4052543755,-4.4531124932

H,0,2.1254840453,-1.0725320551,-1.1648997746

H,0,0.9549042758,-0.6459406165,-2.475382476

H,0,2.4324918594,-1.5989785131,-2.8675511314

H,0,4.6556332917,1.9568151871,-3.2937244941

H,0,3.2242567244,2.8955334491,-2.8246377382

H,0,3.8541772047,1.2903237882,-6.1572571239

H,0,4.5290565971,2.8141485694,-6.8388227549

H,0,5.4345265528,1.927183715,-5.5614518551

H,0,5.5146443074,3.9333237428,-4.2142054728

H,0,4.6425926308,4.7947810802,-5.5322009395

H,0,3.9972970971,4.8401770492,-3.8540614191

H,0,2.5569863657,4.0719490193,-6.2801838822

H,0,1.8774091882,2.4842155469,-5.7975553936

H,0,1.013018573,3.4600782485,-3.6440277413

H,0,1.6145465724,6.0502612092,-5.2258405304

H,0,0.5228832597,5.8642068517,-3.7223939721

TS B97D/6-31+G **/ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSB97DSS

23 parent ts

B97D/6-31+G**

E(RB97D) = -518.696707820

Zero-point correction= 0.217204 (Hartree/Particle)

Thermal correction to Energy= 0.230198

Thermal correction to Enthalpy= 0.231142

Thermal correction to Gibbs Free Energy= 0.178710

Sum of electronic and ZPE= -518.479504

Sum of electronic and thermal Energies= -518.466510

Sum of electronic and thermal Enthalpies= -518.465566

Sum of electronic and thermal Free Energies= -518.517998

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 144.451 48.161 110.354

C,0,1.9798755105,-0.8480299921,-2.35685013

O,0,2.7658999532,0.3578682374,-2.4711999942

C,0,2.8462504077,0.9061500604,-3.7507819627

C,0,3.5697244056,2.1337729604,-3.7226019974

N,0,3.8383117896,2.879903219,-4.8716463925

C,0,4.6651344623,4.0800776964,-4.5718596487

O,0,2.3213629263,0.3410369967,-4.7334779575

C,0,4.3703824437,2.1500430419,-6.0583060956

C,0,2.1250593563,3.714513854,-5.6625936116

C,0,1.5060686538,4.2578476635,-4.4991536592

C,0,0.9131954857,3.4425081801,-3.57045451

H,0,2.0241358657,-1.1229759336,-1.2965016293

H,0,0.9383953333,-0.665272175,-2.6607616149

H,0,2.4012420778,-1.6520345996,-2.978021079

H,0,3.7935497375,2.6032119331,-2.7707251108

H,0,5.3886830018,1.8003932583,-5.8317502087

H,0,3.7162309963,1.3023643115,-6.2737332094

H,0,4.3913717634,2.8449538743,-6.9066748274

H,0,5.655924055,3.7600682536,-4.2167482385

H,0,4.7661611509,4.6761892301,-5.485414992

H,0,4.1603958243,4.6682563752,-3.7970021005

H,0,2.5577078387,4.3797965994,-6.4114458584

H,0,1.7662626709,2.7514175528,-6.0294709111

H,0,1.686045065,5.3085000717,-4.2548405882

H,0,0.6971081559,2.4000120283,-3.8036829553

H,0,0.5697750689,3.8268883022,-2.6083407169

Cation B98/6-31G */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM2B98SB

parent sm

b98/6-31G*

E(RB98) = -519.297732939

Zero-point correction= 0.241750 (Hartree/Particle)

Thermal correction to Energy= 0.254650

Thermal correction to Enthalpy= 0.255594

Thermal correction to Gibbs Free Energy= 0.202269

Sum of electronic and ZPE= -519.055983

Sum of electronic and thermal Energies= -519.043083

Sum of electronic and thermal Enthalpies= -519.042139

Sum of electronic and thermal Free Energies= -519.095464

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.795	47.061	112.232

C,0,2.0511520949,-0.8384620976,-2.2639335555

O,0,2.7947074989,0.3932776758,-2.4135007396

C,0,2.7792421129,0.9470487766,-3.6192617027

O,0,2.1969559895,0.508328807,-4.5889027448

C,0,3.6197415104,2.2253425322,-3.5664110666

N,0,3.7142066001,2.9929613558,-4.8618557916

C,0,4.4175943779,2.1712294835,-5.9161811474

C,0,4.535297041,4.2292661254,-4.5870102661

C,0,2.3284795708,3.4112466434,-5.4079750519

C,0,1.4709015842,4.1336859804,-4.4083463941

C,0,1.1903226772,5.4377896238,-4.5007330085

H,0,2.1846069419,-1.126600535,-1.2218540184

H,0,0.9955821013,-0.6658870919,-2.487329396

H,0,2.45616358,-1.6014509366,-2.9330890547

H,0,4.6384732172,1.9650009772,-3.2643334111

H,0,3.2092023223,2.8944690506,-2.8056072501

H,0,3.8335953909,1.2716131273,-6.1039749549

H,0,4.4964499314,2.7740422465,-6.8225688936

H,0,5.4136707454,1.9171059896,-5.548424771

H,0,5.5060037646,3.9241537246,-4.1924949591

H,0,4.664779615,4.7711044532,-5.5253173525

H,0,4.0062716472,4.8505911853,-3.8635780573

H,0,2.545216563,4.0393657688,-6.2754247168

H,0,1.8598974626,2.4830581522,-5.7395153558

H,0,1.0140965468,3.5361470811,-3.6203318549

H,0,1.6043484755,6.0612908047,-5.291476956

H,0,0.5220726368,5.9215990963,-3.7928905292

TS B98/6-31G */ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSB98SB

23 parent ts

b98/6-31G*

E(RB98) = -518.778127035

Zero-point correction= 0.224009 (Hartree/Particle)

Thermal correction to Energy= 0.236695

Thermal correction to Enthalpy= 0.237640

Thermal correction to Gibbs Free Energy= 0.185806

Sum of electronic and ZPE= -518.554118

Sum of electronic and thermal Energies= -518.541432

Sum of electronic and thermal Enthalpies= -518.540488

Sum of electronic and thermal Free Energies= -518.592321

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.529	46.748	109.093

C,0,2.0351915029,-0.8199621689,-2.3344432231

O,0,2.7266413509,0.422673644,-2.4552158271

C,0,2.7996908645,0.9343133892,-3.7276172516

C,0,3.439543792,2.2120700238,-3.7180254457

N,0,3.7988004862,2.8993535806,-4.868964433

C,0,4.6858576417,4.0450461523,-4.5744597175

O,0,2.3300928962,0.3195786426,-4.693045269

C,0,4.2975507558,2.1130335139,-6.021546311

C,0,2.1341690469,3.845453199,-5.6946417408

C,0,1.5026782756,4.2656020793,-4.5042407364

C,0,0.98585198,3.3312692607,-3.6439036039

H,0,2.0744628231,-1.0776374792,-1.2735342148

H,0,0.9920362705,-0.7271847763,-2.6572815925

H,0,2.5191146524,-1.6035597215,-2.9276462143

H,0,3.7141424658,2.6565390461,-2.7715624032

H,0,5.303558683,1.7347527723,-5.7993564134

H,0,3.6206238852,1.2785709134,-6.1977229862

H,0,4.3382781019,2.7652465147,-6.8985571399

H,0,5.6412126181,3.6846784938,-4.1728513251

H,0,4.8634408437,4.609089247,-5.4930489118

H,0,4.2010139373,4.6910731773,-3.8384797952

H,0,2.5720488361,4.5735066329,-6.3753021154

H,0,1.795294042,2.9229135515,-6.1616488199

H,0,1.6732859554,5.2831316116,-4.1505973805

H,0,0.7152845933,2.3406726597,-3.9981556954

H,0,0.6543876994,3.5972370402,-2.6421914327

Cation B98/6-31+G* */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM2B98SS

parent sm

b98/6-31+G**

E(RB98) = -519.330102315

Zero-point correction= 0.240167 (Hartree/Particle)

Thermal correction to Energy= 0.253178

Thermal correction to Enthalpy= 0.254123

Thermal correction to Gibbs Free Energy= 0.200411

Sum of electronic and ZPE= -519.089935

Sum of electronic and thermal Energies= -519.076924

Sum of electronic and thermal Enthalpies= -519.075980

Sum of electronic and thermal Free Energies= -519.129691

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.872	47.378	113.045

C,0,2.0450435856,-0.8438261167,-2.2514978415

O,0,2.7855741189,0.3919503897,-2.4110161534

C,0,2.7835625983,0.9389173373,-3.6208642759

O,0,2.2115251152,0.4911307794,-4.5942157179

C,0,3.6232682861,2.2160897102,-3.5711435091

N,0,3.7155216955,2.9917328526,-4.8624738276

C,0,4.4176219765,2.1784979748,-5.9261902622

C,0,4.5421548553,4.2240415271,-4.5779200664

C,0,2.333075693,3.4200709572,-5.4060969951

C,0,1.4772143564,4.1450643922,-4.4058711479

C,0,1.1705343792,5.4433163892,-4.5162274646

H,0,2.1757358284,-1.1187418556,-1.2062100138

H,0,0.9906208736,-0.6757183276,-2.4805952297

H,0,2.4582110355,-1.6106674694,-2.9101233536

H,0,4.6420289956,1.9505571625,-3.2748146264

H,0,3.2181326288,2.879766778,-2.8034282973

H,0,3.8262463555,1.288974103,-6.1357246497

H,0,4.510857665,2.7956918579,-6.8206633625

H,0,5.407189435,1.9067507003,-5.5555549644

H,0,5.5179661186,3.9117792167,-4.2041403895

H,0,4.65717726,4.7816508914,-5.5078953601

H,0,4.0265379934,4.8334094645,-3.8358609827

H,0,2.5519310566,4.0496877214,-6.2715173033

H,0,1.8557547401,2.4981103667,-5.7421620211

H,0,1.038016093,3.5557079056,-3.6022222747

H,0,1.5668265811,6.0606458036,-5.3201575804

H,0,0.5007026797,5.9227274882,-3.8077353292

TS B98/6-31+G **/ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSB98SS

23 parent ts

b98/6-31+G**

E(RB98) = -518.819267263

Zero-point correction= 0.222269 (Hartree/Particle)

Thermal correction to Energy= 0.235138

Thermal correction to Enthalpy= 0.236082

Thermal correction to Gibbs Free Energy= 0.183823

Sum of electronic and ZPE= -518.596999

Sum of electronic and thermal Energies= -518.584129

Sum of electronic and thermal Enthalpies= -518.583185

Sum of electronic and thermal Free Energies= -518.635444

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.551	47.257	109.988

C,0,2.0412593518,-0.8267692261,-2.3008137363

O,0,2.7190278056,0.4260191141,-2.4465444468

C,0,2.8149821644,0.9158214068,-3.7260214799

C,0,3.4390770886,2.2031873612,-3.7276469734

N,0,3.8088367451,2.8904031776,-4.871452986

C,0,4.7039598834,4.0301849209,-4.5710538603

O,0,2.3823501301,0.2702665079,-4.6915996997

C,0,4.2899686952,2.118488755,-6.0416133272

C,0,2.121164167,3.8847659106,-5.7040955003

C,0,1.4958322248,4.2725832317,-4.500377354

C,0,0.9507901039,3.327221729,-3.6660957999

H,0,2.0625881891,-1.0475448506,-1.2322592323

H,0,1.0054493406,-0.7548936703,-2.6478627509

H,0,2.552942135,-1.6181270278,-2.8573736186

H,0,3.6774918205,2.6629131817,-2.7786773971

H,0,5.2797821021,1.6995524141,-5.8213458399

H,0,3.5912812062,1.3119609791,-6.2546053745

H,0,4.3627897419,2.7946387344,-6.8968185888

H,0,5.6641030908,3.6602639015,-4.1909250764

H,0,4.8698339524,4.6082159939,-5.4820486516

H,0,4.2355700886,4.666575482,-3.8173392102

H,0,2.5811594768,4.6272986847,-6.352209248

H,0,1.7879226145,2.9742864537,-6.1964816921

H,0,1.67564128,5.2774920731,-4.1179039433

H,0,0.6787563818,2.3445318943,-4.0402643938

H,0,0.62169422,3.5781238673,-2.660609818

Cation wB97/6-31G */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM2wB97SB

parent sm

wb97/6-31G*

E(RwB97) = -519.414979918

Zero-point correction= 0.245716 (Hartree/Particle)

Thermal correction to Energy= 0.258387

Thermal correction to Enthalpy= 0.259332

Thermal correction to Gibbs Free Energy= 0.206296

Sum of electronic and ZPE= -519.169264

Sum of electronic and thermal Energies= -519.156592

Sum of electronic and thermal Enthalpies= -519.155648

Sum of electronic and thermal Free Energies= -519.208684

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.141	46.124	111.624

C,0,2.027264072,-0.7818090359,-2.2746428635

O,0,2.7964059745,0.4324154631,-2.411527894

C,0,2.7752324748,0.989122438,-3.6139720138

O,0,2.1743214336,0.5576888068,-4.5747646762

C,0,3.6246608842,2.253090682,-3.5759765845

N,0,3.7193050049,2.9940831032,-4.8741495637

C,0,4.4283885243,2.1628687254,-5.9015625403

C,0,4.5257106615,4.2319491902,-4.6175014917

C,0,2.3524997067,3.3934596299,-5.4274080012

C,0,1.4687606399,4.0560766068,-4.4103891753

C,0,1.2017410043,5.3606069905,-4.4307777236

H,0,2.1773223714,-1.1038478471,-1.2440361874

H,0,0.9711804255,-0.5746521922,-2.4672529062

H,0,2.3948508867,-1.5358232078,-2.9756398828

H,0,4.6414302752,1.9859732941,-3.2700271664

H,0,3.2183340121,2.9335539517,-2.8210307355

H,0,3.8567645921,1.2493654465,-6.0687323533

H,0,4.4967454112,2.7431522473,-6.8249303675

H,0,5.4299928937,1.9309849451,-5.5308797365

H,0,5.4936951962,3.942262444,-4.2021057288

H,0,4.6666096827,4.7554447871,-5.5659103248

H,0,3.9834264232,4.8672011451,-3.9138096345

H,0,2.5651588927,4.0640194603,-6.2659872998

H,0,1.901550771,2.4735988762,-5.805539994

H,0,0.9935100093,3.4125129641,-3.6685078846

H,0,1.6389455281,6.023289565,-5.1782074461

H,0,0.5252242481,5.8107295207,-3.7070528244

TS WB97/6-31G */ PCM-TS

home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSwB97SB

23 parent ts

wb97/6-31G*

E(RwB97) = -518.876911794

Zero-point correction= 0.229013 (Hartree/Particle)

Thermal correction to Energy= 0.240985

Thermal correction to Enthalpy= 0.241929

Thermal correction to Gibbs Free Energy= 0.191754

Sum of electronic and ZPE= -518.647899

Sum of electronic and thermal Energies= -518.635927

Sum of electronic and thermal Enthalpies= -518.634983

Sum of electronic and thermal Free Energies= -518.685157

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.220	44.788	105.601

C,0,2.0647973152,-0.8397152466,-2.3884806782

O,0,2.7186324101,0.4262440472,-2.4845413274

C,0,2.7190795111,0.9818967749,-3.7294304435

C,0,3.2515619291,2.3130375028,-3.7040519631

N,0,3.6830072335,2.9465244389,-4.8925948633

C,0,4.5854705612,4.0675706801,-4.572208716

O,0,2.2148794265,0.3970282587,-4.6908063013

C,0,4.2696863181,2.1047983286,-5.9551671426

C,0,2.1813682645,3.7812811284,-5.6941129518

C,0,1.5324294751,4.2953791521,-4.5512289291

C,0,1.2028388577,3.3214392224,-3.6270402817

H,0,2.1473311126,-1.1377865395,-1.3405912436

H,0,1.010449279,-0.7595860105,-2.6747960464

H,0,2.5515527928,-1.5818681297,-3.0301898615

H,0,3.7121043067,2.6571118689,-2.7841855214

H,0,5.2528503125,1.7363985693,-5.6389766098

H,0,3.6040434238,1.2648956983,-6.1534248608

H,0,4.3835485864,2.7163079062,-6.8570555472

H,0,5.4955621267,3.6877227101,-4.0932747124

H,0,4.8467692955,4.59643196,-5.4940217149

H,0,4.0703735543,4.7515208202,-3.8915045191

H,0,2.61885162,4.4537817486,-6.4361190914

H,0,1.787498261,2.8552326542,-6.1218154965

H,0,1.7594197233,5.3097126477,-4.2201704534

H,0,0.7866147028,2.3760155581,-3.9748880605

H,0,0.9635336004,3.5760852505,-2.5933626629

Cation wB97XD/6-31G */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM2wB97XDSB

parent sm

wb97xd/6-31G*

E(RwB97XD) = -519.348291809

Zero-point correction= 0.244927 (Hartree/Particle)

Thermal correction to Energy= 0.257599

Thermal correction to Enthalpy= 0.258543

Thermal correction to Gibbs Free Energy= 0.205559

Sum of electronic and ZPE= -519.103365

Sum of electronic and thermal Energies= -519.090693

Sum of electronic and thermal Enthalpies= -519.089749

Sum of electronic and thermal Free Energies= -519.142733

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.646	46.168	111.515

C,0,2.0403547456,-0.7867962794,-2.2668301088

O,0,2.8041856281,0.4228924401,-2.4216470239

C,0,2.7693074886,0.9853819402,-3.6166718377

O,0,2.1607071269,0.5610826954,-4.5723325102

C,0,3.6131878276,2.2505046315,-3.5772362448

N,0,3.7156704256,2.9935485937,-4.8748035216

C,0,4.4291701538,2.1629293654,-5.901018312

C,0,4.5218658988,4.2309520664,-4.6100797711

C,0,2.3483565629,3.3971941767,-5.436540455

C,0,1.4619365898,4.0613303066,-4.4292966264

C,0,1.2123560028,5.3685965162,-4.4345820445

H,0,2.2309259681,-1.1191490322,-1.2489713514

H,0,0.9795417257,-0.5760891329,-2.4114406418

H,0,2.3744398038,-1.5350992163,-2.9869045452

H,0,4.6264220906,1.9891580328,-3.264507918

H,0,3.2014749402,2.9297894177,-2.8280326271

H,0,3.8556868633,1.2556848434,-6.0776825928

H,0,4.5088583147,2.7453729103,-6.8187167879

H,0,5.4233012587,1.9234806082,-5.5236323095

H,0,5.486786437,3.9412875014,-4.1949099981

H,0,4.6638423405,4.758609696,-5.5526315392

H,0,3.9796012575,4.8610688732,-3.9062359041

H,0,2.5686731507,4.0593743359,-6.2755872844

H,0,1.8999900098,2.4784012293,-5.8112517626

H,0,0.972038497,3.4166768656,-3.7030601209

H,0,1.665440842,6.0358740006,-5.1638445589

H,0,0.5349100498,5.8152606142,-3.7138746023

WB97XD/6-31G */ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSwB97XDSB

glycine allyl TSfreq

wb97xd/6-31G*

E(RwB97XD) = -518.818252298

Zero-point correction= 0.227675 (Hartree/Particle)

Thermal correction to Energy= 0.239819

Thermal correction to Enthalpy= 0.240763

Thermal correction to Gibbs Free Energy= 0.190399

Sum of electronic and ZPE= -518.590577

Sum of electronic and thermal Energies= -518.578434

Sum of electronic and thermal Enthalpies= -518.577489

Sum of electronic and thermal Free Energies= -518.627854

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	150.488	45.456	106.000

C,0,2.0142989125,-0.7958060399,-2.3641659798

O,0,2.711634185,0.4381595342,-2.4762017862

C,0,2.7803116218,0.959587034,-3.7337312741

C,0,3.3875172225,2.2489364786,-3.7178403505

N,0,3.7729411004,2.9115393467,-4.8740432652

C,0,4.6409939234,4.0601898382,-4.575828495

O,0,2.3081801512,0.3582182663,-4.7002946578

C,0,4.3000605232,2.1166898535,-5.9964975015

C,0,2.1295999673,3.8068074742,-5.6969127528

C,0,1.5230595358,4.2431118646,-4.5111421398

C,0,1.1031006121,3.2894966388,-3.6195930458

H,0,2.0513860109,-1.062555839,-1.3076170661

H,0,0.9739551785,-0.692250158,-2.6857291704

H,0,2.492675602,-1.5758891964,-2.9627531652

H,0,3.7234357748,2.6577855144,-2.7763202792

H,0,5.3007313618,1.7451422969,-5.7509659543

H,0,3.6317415666,1.2793626874,-6.182060697

H,0,4.3569695255,2.7561916477,-6.8803461497

H,0,5.5844255383,3.7148927115,-4.1401452366

H,0,4.8414391448,4.6101033469,-5.4966970748

H,0,4.1303378232,4.7155151035,-3.8680122479

H,0,2.5504230853,4.5199078396,-6.4023156174

H,0,1.7907978273,2.8716356812,-6.1371650561

H,0,1.7098087575,5.2584419727,-4.1662084386

H,0,0.7734548698,2.3178212197,-3.9726473748

H,0,0.8309741785,3.5444258826,-2.5988052232

Cation wB97XD/6-31+G **/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM2wB97XDSS

parent sm

wb97xd/6-31+G**

E(RwB97XD) = -519.379062031

Zero-point correction= 0.243470 (Hartree/Particle)

Thermal correction to Energy= 0.256170

Thermal correction to Enthalpy= 0.257114

Thermal correction to Gibbs Free Energy= 0.204264

Sum of electronic and ZPE= -519.135592

Sum of electronic and thermal Energies= -519.122892

Sum of electronic and thermal Enthalpies= -519.121948

Sum of electronic and thermal Free Energies= -519.174798

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 160.749 46.433 111.233

C,0,2.0281293843,-0.7863721771,-2.2529988938

O,0,2.7911535574,0.4252327463,-2.4182452221

C,0,2.7763381389,0.9754952203,-3.6199554132

O,0,2.1828585502,0.5377711058,-4.5808939298

C,0,3.6201820071,2.2391083105,-3.5841410717

N,0,3.7180947506,2.9918551932,-4.8765676076

C,0,4.4323251679,2.1745110928,-5.9143231153

C,0,4.5263986848,4.2269549039,-4.6010660011

C,0,2.3515453701,3.4013178072,-5.4331993999

C,0,1.4676958764,4.0666127736,-4.4238230381

C,0,1.1950947567,5.3702017465,-4.4467400474

H,0,2.2165466026,-1.1064420806,-1.2314422709

H,0,0.9682709699,-0.5766560723,-2.402303379

H,0,2.3672635707,-1.5404796027,-2.9637932876

H,0,4.6339982417,1.9720538635,-3.2787829492

H,0,3.2153167712,2.9129388176,-2.826834865

H,0,3.8559316063,1.2746304928,-6.1146684597

H,0,4.5216477063,2.7741388699,-6.8193230684

H,0,5.4219499736,1.9218569666,-5.5354585774

H,0,5.4959733915,3.9313947338,-4.2028025327

H,0,4.6561110091,4.7689842514,-5.5363793634

H,0,3.9937200527,4.845914149,-3.8810852519

H,0,2.5711564849,4.0658025836,-6.270384143

H,0,1.897328593,2.4863513842,-5.8106609812

H,0,0.9946790378,3.4282521689,-3.6811087802

H,0,1.6314233022,6.0318371689,-5.1906864237

H,0,0.5178984421,5.8140515823,-3.7246549271

TS WB97XD/6-31+G **/ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSwB97SDSS

23 parent ts

wB97xD/6-31+G**

E(RwB97XD) = -518.856711302

Zero-point correction= 0.225781 (Hartree/Particle)

Thermal correction to Energy= 0.238136

Thermal correction to Enthalpy= 0.239081

Thermal correction to Gibbs Free Energy= 0.188120

Sum of electronic and ZPE= -518.630930

Sum of electronic and thermal Energies= -518.618575

Sum of electronic and thermal Enthalpies= -518.617631

Sum of electronic and thermal Free Energies= -518.668591

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 149.433 46.011 107.256

C,0,2.0089085743,-0.79561239,-2.3373730977

O,0,2.7030905924,0.4428211763,-2.4699512709

C,0,2.7909823498,0.9483538925,-3.7322269943

C,0,3.3905335106,2.2426879308,-3.7267149683

N,0,3.786101013,2.9042598198,-4.875669322

C,0,4.6585188323,4.0497433533,-4.5740132981

O,0,2.3466248635,0.3238485041,-4.7004090288

C,0,4.2969821442,2.121217749,-6.0139776092

C,0,2.1132098054,3.8395638969,-5.7066715256

C,0,1.5202629807,4.242477767,-4.5045649932

C,0,1.0848920454,3.273465002,-3.6332181558

H,0,2.0335749313,-1.0341410229,-1.2747892065

H,0,0.9738367892,-0.7005702923,-2.6751366819

H,0,2.5026534426,-1.5844726251,-2.9098300666

H,0,3.6970687527,2.6640778616,-2.7806398626

H,0,5.2868601032,1.7194244731,-5.7733139154

H,0,3.6127157737,1.3042747566,-6.2275258246

H,0,4.3741703217,2.7800141987,-6.880930494

H,0,5.6069886747,3.6997272901,-4.1537250652

H,0,4.8483165322,4.6092953984,-5.49042632

H,0,4.1591718596,4.6991293697,-3.8534976175

H,0,2.5482474309,4.5684301561,-6.3855334972

H,0,1.7838566139,2.9110256268,-6.1662266421

H,0,1.7129216978,5.2474028363,-4.1342723954

H,0,0.755154883,2.3092335149,-4.0058430288

H,0,0.8186094818,3.5117827559,-2.6075591183

Cation wB97X/6-31G */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM2wB97XSB

parent sm

wb97x/6-31G*

E(RwB97X) = -519.373462601

Zero-point correction= 0.245540 (Hartree/Particle)

Thermal correction to Energy= 0.258240

Thermal correction to Enthalpy= 0.259184

Thermal correction to Gibbs Free Energy= 0.206043

Sum of electronic and ZPE= -519.127923

Sum of electronic and thermal Energies= -519.115223

Sum of electronic and thermal Enthalpies= -519.114279

Sum of electronic and thermal Free Energies= -519.167419

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.048	46.151	111.843

C,0,2.0413972326,-0.7945103089,-2.2775796753

O,0,2.8020144345,0.4208797263,-2.4172706499

C,0,2.7761660057,0.9815270416,-3.614571658

O,0,2.1769739038,0.552019516,-4.574329743

C,0,3.6182736522,2.2475186299,-3.5728766926

N,0,3.7144545745,2.9929216119,-4.8678585174

C,0,4.4210593006,2.1642960158,-5.8984892658

C,0,4.5238187865,4.2272672345,-4.6071549332

C,0,2.3472540979,3.3965141857,-5.4199362321

C,0,1.4713200604,4.0779762002,-4.4129364175

C,0,1.203923097,5.38033531,-4.4554815415

H,0,2.2053140473,-1.1214697123,-1.252777242

H,0,0.9837375199,-0.5915271182,-2.454580335

H,0,2.4014523875,-1.542590624,-2.9857592697

H,0,4.6334276738,1.9847267625,-3.2649196212

H,0,3.2090567725,2.9234592662,-2.8183888557

H,0,3.8456045969,1.2573201771,-6.0737022728

H,0,4.49681842,2.7489877275,-6.815984253

H,0,5.4180191156,1.9234187849,-5.5271396299

H,0,5.4905919915,3.9347069384,-4.1963822454

H,0,4.6635044494,4.7544272304,-5.5513226068

H,0,3.9864728796,4.8597352956,-3.9005456411

H,0,2.5613815783,4.0516793529,-6.2672877692

H,0,1.8906290982,2.476035727,-5.7833593078

H,0,0.9988026818,3.4500703046,-3.6591273084

H,0,1.6368531031,6.0299901442,-5.2137302412

H,0,0.5307105387,5.8416025803,-3.7388310749

TS wB97x/6-31G*/PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSwB97xSB

23 parent ts

wb97x/6-31G*

E(RwB97X) = -518.839136984

Zero-point correction= 0.228505 (Hartree/Particle)

Thermal correction to Energy= 0.240607

Thermal correction to Enthalpy= 0.241551

Thermal correction to Gibbs Free Energy= 0.191103

Sum of electronic and ZPE= -518.610632

Sum of electronic and thermal Energies= -518.598530

Sum of electronic and thermal Enthalpies= -518.597586

Sum of electronic and thermal Free Energies= -518.648034

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	150.983	45.169	106.176

C,0,2.0392631875,-0.8147728155,-2.3740740216

O,0,2.7144533461,0.4348897983,-2.4773640026

C,0,2.7513968478,0.9720060946,-3.7287903311

C,0,3.3243847463,2.2800981033,-3.7113197289

N,0,3.7337319621,2.9258125976,-4.880010738

C,0,4.618078319,4.0605140935,-4.5744437174

O,0,2.2637115654,0.3781464254,-4.6914495461

C,0,4.2843844744,2.1094603426,-5.9762166106

C,0,2.1490882964,3.8028944059,-5.6980254947

C,0,1.5275046017,4.2661713676,-4.5289151535

C,0,1.1500940974,3.2999020693,-3.6264192833

H,0,2.0963729801,-1.0974964744,-1.322176329

H,0,0.9932959499,-0.7231490757,-2.6806787815

H,0,2.5232578692,-1.5752239923,-2.9930657919

H,0,3.7181632452,2.6583834982,-2.7774695608

H,0,5.2794771442,1.7414009855,-5.7035561869

H,0,3.6190845848,1.2693981822,-6.1636509746

H,0,4.3622408252,2.7345221309,-6.8699971139

H,0,5.5452505542,3.7007133586,-4.1158090469

H,0,4.8496793674,4.5976663473,-5.4967396119

H,0,4.1055613447,4.7321866191,-3.8824942155

H,0,2.5780584198,4.5002916109,-6.4167462351

H,0,1.790477557,2.8708425981,-6.1336018654

H,0,1.7227000427,5.2821888878,-4.1884173813

H,0,0.786274875,2.3398846711,-3.9823261485

H,0,0.8882677964,3.5507291699,-2.6002821289

Cation wb97x /6-31+G **/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSM2wB97XSS

parent sm

wb97x/6-31+G**

E(RwB97X) = -519.406513476

Zero-point correction= 0.243947 (Hartree/Particle)

Thermal correction to Energy= 0.256704

Thermal correction to Enthalpy= 0.257648

Thermal correction to Gibbs Free Energy= 0.204398

Sum of electronic and ZPE= -519.162567

Sum of electronic and thermal Energies= -519.149810

Sum of electronic and thermal Enthalpies= -519.148866

Sum of electronic and thermal Free Energies= -519.202115

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	161.084	46.401	112.073

C,0,2.0303271615,-0.7932456544,-2.2629029431

O,0,2.7893332396,0.4251491313,-2.4138539885

C,0,2.7816572643,0.9749763353,-3.6170420288

O,0,2.1950482311,0.5332519975,-4.5811868043

C,0,3.6238052887,2.2392881506,-3.5801392237

N,0,3.7171545757,2.9919536905,-4.8712450891

C,0,4.4230255746,2.1726391328,-5.9113250661

C,0,4.5310881444,4.222634355,-4.6010517598

C,0,2.3519503028,3.4036573302,-5.4202875875

C,0,1.4746805726,4.0798359626,-4.4102047577

C,0,1.185798628,5.3785662808,-4.460111764

H,0,2.1835252702,-1.1002987149,-1.230827623

H,0,0.9749544257,-0.5948170487,-2.4560338649

H,0,2.404558453,-1.5503499006,-2.953452863

H,0,4.6393168139,1.9710108415,-3.2780176696

H,0,3.2205933576,2.9111404097,-2.8189980807

H,0,3.8425749403,1.2731078259,-6.1066320635

H,0,4.5091534611,2.7717945099,-6.8181094975

H,0,5.4154091576,1.9181966107,-5.5379464739

H,0,5.5023350703,3.9226097615,-4.2076437806

H,0,4.6587613632,4.7636971997,-5.5384097078

H,0,4.00505958,4.8451724036,-3.8778689603

H,0,2.5676805663,4.0656560813,-6.2619343097

H,0,1.8907047584,2.48896155,-5.7932298057

H,0,1.0147139581,3.45305484,-3.6475083413

H,0,1.605963871,6.0281593719,-5.2253358687

H,0,0.50985797,5.8315155463,-3.7410230775

TSwB97x/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSwB97xSS

23 parent ts

wB97x/6-31+G**

E(RwB97X) = -518.879949446

Zero-point correction= 0.226475 (Hartree/Particle)

Thermal correction to Energy= 0.238794

Thermal correction to Enthalpy= 0.239739

Thermal correction to Gibbs Free Energy= 0.188772

Sum of electronic and ZPE= -518.653474

Sum of electronic and thermal Energies= -518.641155

Sum of electronic and thermal Enthalpies= -518.640211

Sum of electronic and thermal Free Energies= -518.691177

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.846	45.759	107.268

C,0,2.0338231588,-0.8112522384,-2.336653686

O,0,2.6986914702,0.4465865879,-2.4654764794

C,0,2.7658618417,0.9578768879,-3.7267977614

C,0,3.332566666,2.2692221281,-3.7245613077

N,0,3.7502469375,2.9171437834,-4.8826541058

C,0,4.6445145277,4.0438653786,-4.5728059848

O,0,2.3169383227,0.3299635249,-4.6905110387

C,0,4.2765332039,2.1145908315,-6.0008245891

C,0,2.1351735115,3.8504537227,-5.7070808756

C,0,1.5243566719,4.264458023,-4.5164337051

C,0,1.1193381183,3.2756201549,-3.6485257206

H,0,2.0759285181,-1.0587119333,-1.2761012556

H,0,0.9934889097,-0.7357899076,-2.6638915506

H,0,2.5409691455,-1.5810284365,-2.9236091994

H,0,3.68332659,2.6691091754,-2.7825396153

H,0,5.2579420891,1.705619026,-5.7366158451

H,0,3.5884975991,1.3014008166,-6.2208209118

H,0,4.3788804114,2.7640485798,-6.8736853878

H,0,5.5774036564,3.6743581887,-4.1336008491

H,0,4.8645931267,4.5931894915,-5.4900127378

H,0,4.1482762831,4.7095585574,-3.8637992785

H,0,2.5806142571,4.5743109908,-6.3874681113

H,0,1.7869338484,2.9317944044,-6.1765853767

H,0,1.7215515622,5.2667558882,-4.1386112225

H,0,0.7649511152,2.3243689241,-4.0363089111

H,0,0.852852458,3.4999484501,-2.618064493

Cation LC-B97D /6-31G */PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentSMLCB97DSB

parent sm

LC-B97D/6-31G*

E(RB97D) = -518.216650707

Zero-point correction= 0.246785 (Hartree/Particle)

Thermal correction to Energy= 0.258980

Thermal correction to Enthalpy= 0.259924

Thermal correction to Gibbs Free Energy= 0.208322

Sum of electronic and ZPE= -517.969866

Sum of electronic and thermal Energies= -517.957670

Sum of electronic and thermal Enthalpies= -517.956726

Sum of electronic and thermal Free Energies= -518.008329

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.513	45.152	108.607

C,0,1.989353905,-0.6828483473,-2.262528349

O,0,2.7986906503,0.4989901678,-2.4193588055

C,0,2.7496440793,1.0716964133,-3.6018873459

O,0,2.0944100652,0.6792326828,-4.5350597143

C,0,3.6240122751,2.3056134941,-3.5913970923

N,0,3.727002951,3.0014406935,-4.9088994951

C,0,4.4585373694,2.1455042585,-5.8906045163

C,0,4.5100354273,4.2537876781,-4.6763147198

C,0,2.3712543039,3.3773940958,-5.5060133651

C,0,1.432512444,3.8966873563,-4.4655360898

C,0,1.2544763563,5.1898574512,-4.2600055694

H,0,2.1483337983,-1.0140221655,-1.2370355169

H,0,0.9405093128,-0.4312208595,-2.439813655

H,0,2.3127403792,-1.4425635146,-2.9787280122

H,0,4.6366518324,2.0328079359,-3.283583681

H,0,3.2218815991,3.0134588224,-2.8624670364

H,0,3.902178674,1.2158475755,-6.0127811366

H,0,4.5108389442,2.6911211376,-6.8353126117

H,0,5.4615690488,1.958152212,-5.5007689291

H,0,5.4609673234,3.9858121876,-4.2108134917

H,0,4.6777906636,4.7312808185,-5.6435248562

H,0,3.9250346931,4.904850131,-4.0234814896

H,0,2.594761528,4.1318030612,-6.2648406009

H,0,1.9856088945,2.4759782427,-5.977601708

H,0,0.9036311499,3.1509024453,-3.8743743508

H,0,1.7855263223,5.9281617676,-4.8600468803

H,0,0.5710780094,5.5575922583,-3.4995439812

TS LC-B97D/6-31G */ PCM-TS

/home/bibaswanbiswas/c8/Parentcalcs/b97family/23parentTSLCB97DSB

23 parent ts

LC-B97D/6-31G*

E(RB97D) = -517.680577010

Zero-point correction= 0.229305 (Hartree/Particle)

Thermal correction to Energy= 0.241036

Thermal correction to Enthalpy= 0.241980

Thermal correction to Gibbs Free Energy= 0.192564

Sum of electronic and ZPE= -517.451272

Sum of electronic and thermal Energies= -517.439541

Sum of electronic and thermal Enthalpies= -517.438597

Sum of electronic and thermal Free Energies= -517.488013

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.252	44.463	104.005

C,0,1.8665656953,-0.7084827635,-2.4386998118

O,0,2.7072902216,0.4380079121,-2.5108465806

C,0,2.8305665286,0.981802071,-3.7444684079

C,0,3.4680533718,2.2485069801,-3.7029343693

N,0,3.8173604732,2.9064894862,-4.867086469

C,0,4.5801502552,4.1242225241,-4.601073593

O,0,2.3289673586,0.4403776491,-4.72662376

C,0,4.3831357478,2.1523017176,-5.9906338484

C,0,2.0640614183,3.6501951248,-5.6729481568

C,0,1.5315939855,4.1365281349,-4.4863810902

C,0,1.2503823742,3.2089393585,-3.5146804522

H,0,1.852616292,-1.0084835273,-1.389196827

H,0,0.8548262135,-0.4608072811,-2.7797978123

H,0,2.2581655607,-1.5169304356,-3.0638956091

H,0,3.8577381941,2.6213448109,-2.7657876336

H,0,5.4227679257,1.8803089802,-5.7668983737

H,0,3.7830916724,1.2594428242,-6.1561559108

H,0,4.3548983786,2.7962751437,-6.8761667047

H,0,5.5579600816,3.8656544844,-4.1749070445

H,0,4.7135253983,4.6709601629,-5.5391002976

H,0,4.0165369452,4.7403206388,-3.8945069468

H,0,2.4484842482,4.3164887052,-6.4432050277

H,0,1.7812815192,2.6502386321,-6.0002687691

H,0,1.7270445248,5.1708646613,-4.2064555611

H,0,0.8767705219,2.2298102864,-3.7999240743

H,0,1.0804190939,3.503084719,-2.4813968683

Cation- B3LYP /6-31+G/PCM-Conf2**

/home/bibaswanbiswas/c8/Parentcalcs/23parentSM2B3LYPSS

parent sm

B3LYP/6-31+G**

E(RB3LYP) = -519.536967748

Zero-point correction= 0.240197 (Hartree/Particle)

Thermal correction to Energy= 0.253276

Thermal correction to Enthalpy= 0.254221

Thermal correction to Gibbs Free Energy= 0.199879

Sum of electronic and ZPE= -519.296770

Sum of electronic and thermal Energies= -519.283691

Sum of electronic and thermal Enthalpies= -519.282747

Sum of electronic and thermal Free Energies= -519.337089

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.933	47.446	114.371

C,0,2.0567111022,-0.8679876245,-2.2528599574

O,0,2.796051203,0.3733597139,-2.4118368817

C,0,2.7866344848,0.9295161946,-3.6201584389

O,0,2.2101830471,0.4845457872,-4.5935833724

C,0,3.6191443785,2.2068828839,-3.5671505481

N,0,3.7107970344,2.9914219293,-4.8544286647

C,0,4.4103552921,2.1838482363,-5.9250945069

C,0,4.5409646282,4.2207797237,-4.5643798171

C,0,2.3262510403,3.4247968442,-5.3935402348

C,0,1.4863126127,4.1776356596,-4.4056544417

C,0,1.1679050496,5.4671008014,-4.554365488

H,0,2.1935558471,-1.1452895965,-1.2100951562

H,0,1.0021855652,-0.7004035175,-2.4761365337

H,0,2.4682535926,-1.6301854027,-2.9159062534

H,0,4.6375253279,1.9449305258,-3.2716426849

H,0,3.2132958016,2.8646222135,-2.7970340897

H,0,3.8146491992,1.3023683994,-6.1476028198

H,0,4.5123832558,2.8093184031,-6.811184128

H,0,5.3951058772,1.9001245027,-5.5543718602

H,0,5.5183560127,3.9047600312,-4.201976995

H,0,4.6488202376,4.7870184544,-5.4884684017

H,0,4.0330690572,4.8230334041,-3.8135731996

H,0,2.5436130135,4.0329539254,-6.2726125778

H,0,1.839026617,2.5017043708,-5.7069289851

H,0,1.065428755,3.6148788878,-3.5752533719

H,0,1.5457673256,6.0597966939,-5.3838872164

H,0,0.5066866416,5.9657865549,-3.8525963752

TS- B3LYP/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/23parentTSB3LYPSS

23 parent ts

B3LYP/6-31+G**

E(RB3LYP) = -519.030461902

Zero-point correction= 0.222429 (Hartree/Particle)

Thermal correction to Energy= 0.235288

Thermal correction to Enthalpy= 0.236233

Thermal correction to Gibbs Free Energy= 0.183971

Sum of electronic and ZPE= -518.808033

Sum of electronic and thermal Energies= -518.795173

Sum of electronic and thermal Enthalpies= -518.794229

Sum of electronic and thermal Free Energies= -518.846491

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.646	47.282	109.994

C,0,2.0464163806,-0.8404928319,-2.3029579915

O,0,2.7308080223,0.4128404119,-2.4453893647

C,0,2.8273741842,0.9117607462,-3.7266111398

C,0,3.4654026925,2.1860789655,-3.7255076312

N,0,3.8208471062,2.8832849213,-4.8665259223

C,0,4.7132744981,4.0259671603,-4.5688935975

O,0,2.385320975,0.2721326076,-4.6948047545

C,0,4.2960271129,2.1187232574,-6.0443986626

C,0,2.1168394678,3.8755825629,-5.6983323958

C,0,1.4889082395,4.2807756554,-4.5022817705

C,0,0.9065949286,3.3672315433,-3.6656474406

H,0,2.0705016078,-1.0656095875,-1.2364122536

H,0,1.0109504262,-0.7627408857,-2.6459924636

H,0,2.5524331476,-1.6306357383,-2.864208327

H,0,3.6923551141,2.6497326321,-2.7772679816

H,0,5.2871383863,1.7019403186,-5.831547437

H,0,3.5995235294,1.3120250644,-6.2565750038

H,0,4.3628180595,2.7974072509,-6.8962440417

H,0,5.6789058711,3.6583667551,-4.2041153657

H,0,4.8653966213,4.6111560314,-5.4760087306

H,0,4.2529195316,4.6535375176,-3.8050270754

H,0,2.5806312337,4.6083004309,-6.3521704184

H,0,1.7818858019,2.9624588415,-6.1804654629

H,0,1.6691797097,5.2912043751,-4.1376569459

H,0,0.6507166766,2.372773325,-4.0152556285

H,0,0.5610846756,3.643659669,-2.673742193

TS- UB3LYP/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/tsUB3BBPCM

sean allyl ester checking ts for u instability

UB3LYP/6-31+G**

E(UB3LYP) = -519.030461924

Zero-point correction= 0.222428 (Hartree/Particle)

Thermal correction to Energy= 0.235288

Thermal correction to Enthalpy= 0.236232

Thermal correction to Gibbs Free Energy= 0.183970

Sum of electronic and ZPE= -518.808034

Sum of electronic and thermal Energies= -518.795174

Sum of electronic and thermal Enthalpies= -518.794230

Sum of electronic and thermal Free Energies= -518.846492

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 147.646 47.283 109.995

C,0,2.047329036,-0.8406727389,-2.3028548348

O,0,2.7309139453,0.4131264398,-2.4450550182

C,0,2.8281345915,0.9117958482,-3.7263243397

C,0,3.4652710447,2.1865658354,-3.7250375863

N,0,3.8208861261,2.8837848455,-4.8659889232

C,0,4.7121228876,4.0273148946,-4.5680549793

O,0,2.387296342,0.2716067618,-4.6947099101

C,0,4.2975640363,2.1193084221,-6.0433107027

C,0,2.1166392585,3.8743420473,-5.6992785075

C,0,1.4875970393,4.2797034653,-4.5038563906

C,0,0.9052483996,3.3662262677,-3.667178332

H,0,2.0707028621,-1.0654902546,-1.2362301607

H,0,1.0120884651,-0.7637757561,-2.6467620919

H,0,2.5543888488,-1.6305924017,-2.8634787924

H,0,3.6910951999,2.6506593498,-2.7767433707

H,0,5.2888856181,1.7034435374,-5.8296467996

H,0,3.6019095276,1.3119464055,-6.2557469716

H,0,4.3643700568,2.7978070455,-6.8953023339

H,0,5.6778752369,3.6606342205,-4.2026724884

H,0,4.8642304205,4.6124870415,-5.4751830084

H,0,4.2507787726,4.6546005885,-3.8045531044

H,0,2.5802828342,4.6070790157,-6.3531957333

H,0,1.7826712835,2.9607167835,-6.1811562034

H,0,1.6668758242,5.2904577714,-4.1396453837

H,0,0.6502713104,2.371407809,-4.0163929492

H,0,0.5588250323,3.6429777555,-2.6756810841

Cation- M06/6-31+G/PCM-Conf2**

/home/bibaswanbiswas/c8/Parentcalcs/23parentSM2M06SS

parent sm

M06/6-31+G**

E(RM06) = -519.180677407

Zero-point correction= 0.239200 (Hartree/Particle)

Thermal correction to Energy= 0.251979

Thermal correction to Enthalpy= 0.252923

Thermal correction to Gibbs Free Energy= 0.200158

Sum of electronic and ZPE= -518.941477

Sum of electronic and thermal Energies= -518.928698

Sum of electronic and thermal Enthalpies= -518.927754

Sum of electronic and thermal Free Energies= -518.980519

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	158.119	47.201	111.054

C,0,2.0548077151,-0.8069902191,-2.2666049013

O,0,2.8042002784,0.4132329487,-2.4169704966

C,0,2.7767769764,0.9741099188,-3.6145031516

O,0,2.1789685075,0.5448848039,-4.5756764332

C,0,3.6117059705,2.234379581,-3.5719550411

N,0,3.7059292067,2.9892979165,-4.8615985659

C,0,4.4132653722,2.1714935893,-5.9030286037

C,0,4.5220684648,4.2184481893,-4.5911351054

C,0,2.3363538577,3.4068587399,-5.4182216501

C,0,1.4685027424,4.0941182983,-4.4220648267

C,0,1.2035284449,5.3984864012,-4.4817630139

H,0,2.2212763118,-1.1280261754,-1.2401402504

H,0,0.9941604072,-0.6152356987,-2.4434531556

H,0,2.4205114662,-1.5582436038,-2.9699646958

H,0,4.6313822239,1.9732069988,-3.2679626584

H,0,3.2109844681,2.9064684808,-2.8059489456

H,0,3.8331762872,1.270505657,-6.1036627102

H,0,4.5018498274,2.7754423874,-6.8082184424

H,0,5.4062535888,1.9163463418,-5.5270639405

H,0,5.4974961666,3.9149976588,-4.2064444092

H,0,4.6421597563,4.7641830166,-5.5287204052

H,0,4.0035202716,4.8397068741,-3.8590811267

H,0,2.5659587835,4.0587900065,-6.2673954754

H,0,1.8777191292,2.4867097177,-5.7875349027

H,0,0.9930654158,3.4773129776,-3.6584156872

H,0,1.6432417987,6.0330394061,-5.2506616709

H,0,0.530168561,5.8737937869,-3.7741327345

TS-M06/6-31+G/PCM**

/home/bibaswanbiswas/c8/Parentcalcs/23parentTSM06SS

23 parent ts

M06/6-31+G**

E(RM06) = -518.672218980

Zero-point correction= 0.221419 (Hartree/Particle)

Thermal correction to Energy= 0.234073

Thermal correction to Enthalpy= 0.235017

Thermal correction to Gibbs Free Energy= 0.183564

Sum of electronic and ZPE= -518.450800

Sum of electronic and thermal Energies= -518.438146

Sum of electronic and thermal Enthalpies= -518.437202

Sum of electronic and thermal Free Energies= -518.488655

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	146.883	47.194	108.293

C,0,1.9671225433,-0.7456365185,-2.3212418089

O,0,2.7121118167,0.4575732541,-2.4580435898

C,0,2.8440248132,0.9307112903,-3.732700632

C,0,3.4751729877,2.2072828396,-3.7317548961

N,0,3.8260521409,2.8911200613,-4.8750453534

C,0,4.6869114038,4.0455297489,-4.5899015879

O,0,2.4203389841,0.2898949598,-4.6977734322

C,0,4.3115944948,2.1371405277,-6.0405883066

C,0,2.0913624163,3.8466371973,-5.6885836532

C,0,1.5051064714,4.2034505334,-4.47035176

C,0,1.0287798396,3.2294026594,-3.6338746784

H,0,1.9471634658,-0.9677734744,-1.2533398869

H,0,0.9449958083,-0.6159793616,-2.6939085579

H,0,2.4399600841,-1.5706304821,-2.8634277195

H,0,3.7157110883,2.6684792338,-2.7808011922

H,0,5.3160508015,1.7448935292,-5.832348679

H,0,3.6342971012,1.3108832667,-6.2522231421

H,0,4.3585222749,2.814341629,-6.8985471319

H,0,5.660634486,3.7030408787,-4.2154868607

H,0,4.8331125829,4.6257257532,-5.5046068256

H,0,4.2105695377,4.6764772218,-3.83445581

H,0,2.5305003811,4.5955002016,-6.34566916

H,0,1.7864595411,2.9165570342,-6.1672448899

H,0,1.6757988694,5.2073624813,-4.0784145853

H,0,0.755718025,2.2514859249,-4.0250261538

H,0,0.7361820408,3.44399061,-2.6086797064

Cation/ APFD/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2APFDPCMSB

parent sm conf 2

APFD/6-31G*

E(RAPFD) = -519.085647732

Zero-point correction= 0.242905 (Hartree/Particle)

Zero-point correction= 0.242996 (Hartree/Particle)

Thermal correction to Energy= 0.255824

Thermal correction to Enthalpy= 0.256768

Thermal correction to Gibbs Free Energy= 0.203415

Sum of electronic and zero-point Energies= -518.842652

Sum of electronic and thermal Energies= -518.829824

Sum of electronic and thermal Enthalpies= -518.828880

Sum of electronic and thermal Free Energies= -518.882233

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	160.532	46.701	112.290

C,0,2.0183189617,-0.7563565164,-2.2586730326

O,0,2.783518533,0.4524034038,-2.4162229495

C,0,2.7726308215,0.990634896,-3.6254178874

O,0,2.1802290993,0.5560312753,-4.5893280946

C,0,3.6274444359,2.248747365,-3.5886001182

N,0,3.724240861,2.9927182072,-4.8841586239

C,0,4.4336071642,2.1683038338,-5.9128069429

C,0,4.5221686616,4.2309961967,-4.6201075918

C,0,2.3519752871,3.3926952127,-5.4379188305

C,0,1.4611410001,4.0278132734,-4.4203097719

C,0,1.2125089887,5.3376025827,-4.3961435796

H,0,2.148582737,-1.0447555898,-1.2176588233

H,0,0.9664810655,-0.5634547827,-2.4784109112

H,0,2.4015097069,-1.5307037398,-2.9260566854

H,0,4.642483961,1.9820335843,-3.2834641281

H,0,3.2264065853,2.9326792008,-2.8367244642

H,0,3.8735290519,1.2491854106,-6.0709807328

H,0,4.4876566496,2.7439202271,-6.8371083068

H,0,5.4386792253,1.9496631447,-5.5509136004

H,0,5.4847540738,3.9470314827,-4.1949516377

H,0,4.6709763197,4.7542775452,-5.564401883

H,0,3.9690042536,4.8623971795,-3.925276023

H,0,2.5680434967,4.0716730628,-6.265397622

H,0,1.9161958184,2.4742042832,-5.8307330849

H,0,0.9671782519,3.3652974542,-3.7112520088

H,0,1.6693150965,6.0208992862,-5.1090504213

H,0,0.5304518925,5.7713805207,-3.6702552443

TS/ APFD /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSAPFDPCMSB

parent ts exo s-cis

APFD/6-31G*

E(RAPFD) = -518.566897926

Zero-point correction= 0.225645 (Hartree/Particle)

Thermal correction to Energy= 0.237974

Thermal correction to Enthalpy= 0.238919

Thermal correction to Gibbs Free Energy= 0.188069

Sum of electronic and ZPE= -518.341253

Sum of electronic and thermal Energies= -518.328924

Sum of electronic and thermal Enthalpies= -518.327979

Sum of electronic and thermal Free Energies= -518.378829

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.331	46.128	107.023

C,0,1.9999359942,-0.7903283736,-2.3782242315

O,0,2.724075863,0.4282193717,-2.4803738468

C,0,2.7932427007,0.9588664256,-3.7396778803

C,0,3.4471177992,2.2200405452,-3.7171421347

N,0,3.7906714559,2.902620653,-4.8711210136

C,0,4.6445197283,4.0610883551,-4.5793847854

O,0,2.2970650728,0.3821402607,-4.7136473317

C,0,4.3177508345,2.121031544,-6.001274973

C,0,2.1296616196,3.7761281229,-5.6826316634

C,0,1.5216866715,4.2387279153,-4.5008074724

C,0,1.0648429184,3.3165133145,-3.5990562224

H,0,2.0420203736,-1.0731350642,-1.3253564313

H,0,0.957625708,-0.6606409401,-2.6871834842

H,0,2.4517285474,-1.5749545574,-2.9932142948

H,0,3.7491126643,2.6509222832,-2.7736548576

H,0,5.3328072622,1.7806811562,-5.769042725

H,0,3.6691185765,1.2642236736,-6.1693754564

H,0,4.3401269643,2.7583378302,-6.8883837478

H,0,5.598417391,3.7249494313,-4.1587574329

H,0,4.8254445606,4.618514077,-5.4998888252

H,0,4.1336678089,4.7045138586,-3.86065706

H,0,2.5457282208,4.4748511898,-6.4058321653

H,0,1.7885709799,2.8312582183,-6.1005542062

H,0,1.6947151192,5.2671323759,-4.1841812319

H,0,0.7803345964,2.3212922128,-3.9259764806

H,0,0.7742645687,3.5944671207,-2.5886400456

Cation-B3LYPGD2/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2B3LYPPCMSBGD2

parent sm conf 2

B3LYP/6-31G*

E(RB3LYP) = -519.541373957

Zero-point correction= 0.241730 (Hartree/Particle)

Thermal correction to Energy= 0.254499

Thermal correction to Enthalpy= 0.255443

Thermal correction to Gibbs Free Energy= 0.202324

Sum of electronic and zero-point Energies= -519.299644

Sum of electronic and thermal Energies= -519.286875

Sum of electronic and thermal Enthalpies= -519.285931

Sum of electronic and thermal Free Energies= -519.339050

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	159.700	46.763	111.799

C,0,2.0243628679,-0.7919076275,-2.2532830939

O,0,2.7865950862,0.433093851,-2.4083865448

C,0,2.7742874194,0.9772896663,-3.6200782559

O,0,2.1850053133,0.5363738108,-4.5857019749

C,0,3.6207420756,2.2452731397,-3.5782450973

N,0,3.7189823465,2.9936657389,-4.8805134428

C,0,4.4358886691,2.1676469014,-5.9167961454

C,0,4.5225235979,4.2396631405,-4.6137503115

C,0,2.3385480653,3.3982602508,-5.4408430236

C,0,1.4630749419,4.0570411579,-4.4204759789

C,0,1.2142234089,5.3679042803,-4.4239178528

H,0,2.1579478252,-1.0801010673,-1.2111689693

H,0,0.9719318482,-0.6007518815,-2.4773951853

H,0,2.4169941438,-1.5573120149,-2.9273356856

H,0,4.6386395063,1.9888258649,-3.2746498205

H,0,3.206984996,2.9282181215,-2.8331777256

H,0,3.8570528482,1.2632670978,-6.0940687402

H,0,4.510977935,2.764922138,-6.826837298

H,0,5.4299227803,1.9305181398,-5.5336768218

H,0,5.4903540485,3.9443468648,-4.2061509834

H,0,4.6502483999,4.765782228,-5.5604776327

H,0,3.9721274981,4.8580057597,-3.9044527152

H,0,2.5634059103,4.0666819261,-6.2744082265

H,0,1.8980259783,2.4744892804,-5.8135487545

H,0,0.99476643,3.4102260052,-3.6818103797

H,0,1.6569719606,6.0269948334,-5.1680700052

H,0,0.5484460989,5.8189003941,-3.6931023349

TS/ B3LYPGD2 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSB3LYPPCMSBGD2

parent ts exo s-cis

B3LYP/6-31G*

E(RB3LYP) = -519.022559409

Zero-point correction= 0.223789 (Hartree/Particle)

Thermal correction to Energy= 0.236342

Thermal correction to Enthalpy= 0.237287

Thermal correction to Gibbs Free Energy= 0.185860

Sum of electronic and ZPE= -518.798770

Sum of electronic and thermal Energies= -518.786217

Sum of electronic and thermal Enthalpies= -518.785273

Sum of electronic and thermal Free Energies= -518.836700

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.307	46.622	108.237

C,0,1.9841384717,-0.8034473331,-2.3646308064

O,0,2.7305885842,0.4133293752,-2.4658945835

C,0,2.8094879254,0.9454087977,-3.7311980735

C,0,3.4880055004,2.197521651,-3.7104448392

N,0,3.8269326628,2.8868539471,-4.8594396022

C,0,4.6582953075,4.0715292515,-4.5795028541

O,0,2.3061396933,0.3691158586,-4.705045214

C,0,4.336690105,2.1240451039,-6.0181670759

C,0,2.1022583012,3.781443345,-5.6952081653

C,0,1.5171272083,4.2363656361,-4.5009133427

C,0,1.0294298577,3.3281291338,-3.5984179891

H,0,2.0219181727,-1.0864147652,-1.310154135

H,0,0.9450218547,-0.6537457208,-2.6792861075

H,0,2.4285853592,-1.5899645775,-2.9844391755

H,0,3.7639138356,2.6396956,-2.7647136647

H,0,5.3549129896,1.7746496052,-5.8048097841

H,0,3.6780988972,1.2763819795,-6.1963593004

H,0,4.3485243365,2.788623082,-6.8863113399

H,0,5.6298919205,3.758149816,-4.1776342263

H,0,4.8017149926,4.6310221409,-5.5063804205

H,0,4.1384763177,4.696803853,-3.8497345584

H,0,2.5377515118,4.4768759158,-6.4079743698

H,0,1.7830612279,2.8236241043,-6.0977192485

H,0,1.7001065178,5.2629118754,-4.1852737898

H,0,0.7581176035,2.3284396361,-3.9210927846

H,0,0.7350648453,3.6201136888,-2.5932945491

Cation/ PBEGD2/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2PBEPCMSBGD2

parent sm conf 2

PBEPBE/6-31G*

E(RPBE-PBE) = -518.871680499

Zero-point correction= 0.234868 (Hartree/Particle)

Thermal correction to Energy= 0.247970

Thermal correction to Enthalpy= 0.248915

Thermal correction to Gibbs Free Energy= 0.195083

Sum of electronic and zero-point Energies= -518.636813

Sum of electronic and thermal Energies= -518.623710

Sum of electronic and thermal Enthalpies= -518.622766

Sum of electronic and thermal Free Energies= -518.676598

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	155.604	48.161	113.299

C,0,2.0157960413,-0.8005460685,-2.259521803

O,0,2.7753264908,0.434631849,-2.3930369619

C,0,2.7876740065,0.9638435832,-3.6232436459

O,0,2.222020114,0.4992189312,-4.6047580961

C,0,3.630211618,2.2393272993,-3.5740167089

N,0,3.7218534521,2.993383041,-4.8777132949

C,0,4.4351039459,2.1714566594,-5.9220547593

C,0,4.5192011544,4.2450448066,-4.6121206001

C,0,2.3280139852,3.3889722174,-5.4245152391

C,0,1.4696399951,4.071823844,-4.4044688026

C,0,1.2173594287,5.3910903066,-4.4363321089

H,0,2.1231660248,-1.0878851992,-1.2059393391

H,0,0.9604244096,-0.6184223603,-2.5155440767

H,0,2.4350771446,-1.5703324189,-2.9259240829

H,0,4.6590413274,1.9876644927,-3.2707131399

H,0,3.2137805644,2.926878081,-2.8211485489

H,0,3.8553733265,1.2562010875,-6.0939930484

H,0,4.4984008316,2.773090478,-6.8399194091

H,0,5.4419370056,1.9390959301,-5.5462570314

H,0,5.496613589,3.9537527109,-4.2024603633

H,0,4.6450457925,4.7765712267,-5.5657200612

H,0,3.9619987634,4.866264485,-3.8972117085

H,0,2.5420656573,4.0418079645,-6.2845928805

H,0,1.8814734555,2.4461685702,-5.7709866017

H,0,1.0050790963,3.4389682206,-3.6386228657

H,0,1.6516186757,6.0368741308,-5.2088701392

H,0,0.5557361033,5.8623741312,-3.7026376832

TS/ PBEGD2 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSPBEPCMSBGD2

parent ts exo s-cis

PBEPBE/6-31G*

E(RPBE-PBE) = -518.366686658

Zero-point correction= 0.217743 (Hartree/Particle)

Thermal correction to Energy= 0.230580

Thermal correction to Enthalpy= 0.231524

Thermal correction to Gibbs Free Energy= 0.179576

Sum of electronic and ZPE= -518.148943

Sum of electronic and thermal Energies= -518.136107

Sum of electronic and thermal Enthalpies= -518.135163

Sum of electronic and thermal Free Energies= -518.187111

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 144.691 47.902 109.334

Charge = 0 Multiplicity = 1

Redundant internal coordinates found in file.

C,0,1.9839941672,-0.8238953816,-2.3879762833

O,0,2.7462379833,0.3909225266,-2.4619780914

C,0,2.8138799616,0.9415034663,-3.7339240465

C,0,3.512256651,2.186830635,-3.7029674964

N,0,3.8217363723,2.8933790112,-4.8604243743

C,0,4.6485280814,4.086594473,-4.580972098

O,0,2.2895198387,0.3793309889,-4.7176634904

C,0,4.3444002213,2.1253717268,-6.0155616537

C,0,2.1290251253,3.7348790411,-5.6796562045

C,0,1.5228969361,4.248239435,-4.5060652547

C,0,1.0093374492,3.3800916472,-3.5722620424

H,0,2.0312180916,-1.1383415507,-1.334552077

H,0,0.9343110498,-0.6555191317,-2.6883834426

H,0,2.4129977755,-1.6053567766,-3.0396206638

H,0,3.7778943679,2.6441416502,-2.7515215968

H,0,5.3774909427,1.7995882649,-5.7988545657

H,0,3.694596986,1.2546422646,-6.1730464772

H,0,4.3362173385,2.7806279924,-6.9009857084

H,0,5.6283446134,3.7745595685,-4.1777785109

H,0,4.7878866182,4.6514458441,-5.5147817265

H,0,4.1208244515,4.7112693644,-3.8440656529

H,0,2.5517500004,4.4083759268,-6.43401332

H,0,1.7872167351,2.760957932,-6.0499889163

H,0,1.6988089994,5.2975108385,-4.2346079485

H,0,0.7581669772,2.3531434205,-3.8539257808

H,0,0.6947162655,3.7171678227,-2.5784625765

Cation/ BLYPGD2/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2BLYPPCMSBGD2

parent sm conf 2

BLYP/6-31G*

E(RB-LYP) = -519.318058822

Zero-point correction= 0.233919 (Hartree/Particle)

Thermal correction to Energy= 0.247103

Thermal correction to Enthalpy= 0.248047

Thermal correction to Gibbs Free Energy= 0.193936

Sum of electronic and zero-point Energies= -519.084140

Sum of electronic and thermal Energies= -519.070956

Sum of electronic and thermal Enthalpies= -519.070011

Sum of electronic and thermal Free Energies= -519.124123

E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	155.060	48.455	113.887

C,0,2.0041728129,-0.8228240244,-2.2375598515

O,0,2.7734811555,0.4229584498,-2.384605604

C,0,2.7817368085,0.9561892662,-3.6206278081

O,0,2.2091801894,0.4958601335,-4.6033807637

C,0,3.6338781119,2.2364996479,-3.5697890405

N,0,3.7286346218,2.9976305148,-4.884480686

C,0,4.449995304,2.1687442835,-5.9376990194

C,0,4.5348108986,4.2593863449,-4.6143772208

C,0,2.3214234254,3.4022957897,-5.4428439441

C,0,1.4551135414,4.0745368314,-4.4130876063

C,0,1.2034998329,5.3957209692,-4.4281312122

H,0,2.1201118612,-1.1002658804,-1.1826406054

H,0,0.9495980107,-0.6349433884,-2.4898350781

H,0,2.4210012842,-1.5930936639,-2.903881832

H,0,4.6617394072,1.9826980773,-3.2714756431

H,0,3.217062738,2.925539828,-2.821724227

H,0,3.8674833378,1.2570710113,-6.109101532

H,0,4.5137861055,2.7749741947,-6.851305808

H,0,5.4536038395,1.9370730388,-5.5554789269

H,0,5.5091528003,3.9615408786,-4.2047158583

H,0,4.6592040139,4.7875739605,-5.5687708317

H,0,3.9748740318,4.8759525996,-3.8998753832

H,0,2.5459508845,4.0650933113,-6.290209379

H,0,1.8832056282,2.4625837774,-5.7998416262

H,0,0.9957832088,3.4307209426,-3.6556577273

H,0,1.6384876266,6.049803116,-5.1917726866

H,0,0.5420605193,5.8579979901,-3.6894530992

TS/ BLYPGD2 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSBLYPPCMSBGD2

parent ts exo s-cis

BLYP/6-31G*

E(RB-LYP) = -518.811650515

Zero-point correction= 0.216786 (Hartree/Particle)

Thermal correction to Energy= 0.229707

Thermal correction to Enthalpy= 0.230651

Thermal correction to Gibbs Free Energy= 0.178524

Sum of electronic and ZPE= -518.594865

Sum of electronic and thermal Energies= -518.581944

Sum of electronic and thermal Enthalpies= -518.580999

Sum of electronic and thermal Free Energies= -518.633126

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 144.143 48.136 109.711

C,0,1.9450451684,-0.830533539,-2.3951735216

O,0,2.7697226486,0.3574345904,-2.4680368836

C,0,2.8434892981,0.9344973867,-3.7423573283

C,0,3.6039148659,2.1415029095,-3.7040441176

N,0,3.8557261059,2.8869726922,-4.8635268064

C,0,4.6582032905,4.1119035536,-4.5823143321

O,0,2.2779407524,0.4101393278,-4.7310462835

C,0,4.3946112479,2.1436322123,-6.0455983809

C,0,2.1186771046,3.6650252288,-5.6545507253

C,0,1.5045188163,4.2291469374,-4.4966712143

C,0,0.9477473192,3.4214647168,-3.5371045034

H,0,1.9997791953,-1.1612335012,-1.3471694754

H,0,0.8997680792,-0.6052622985,-2.6718462477

H,0,2.324243255,-1.6192484136,-3.0680275947

H,0,3.85450302,2.6048007489,-2.7529712644

H,0,5.4354475643,1.8424688055,-5.8349196462

H,0,3.7643413756,1.2624096925,-6.2107489736

H,0,4.3634858091,2.8143074222,-6.9179121175

H,0,5.6532857225,3.8210011305,-4.2037005386

H,0,4.7590680101,4.6890046122,-5.5124521018

H,0,4.1245661842,4.7068148015,-3.8270799235

H,0,2.5231184535,4.3140257226,-6.4372001446

H,0,1.7831924062,2.6753770674,-5.9786739852

H,0,1.6663827717,5.2928985009,-4.2832253784

H,0,0.7394087313,2.3708296823,-3.7513726391

H,0,0.6040668045,3.8180810102,-2.5763158721

Cation/ BP86GD2/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2BP86PCMSBGD2

parent sm conf 2

BP86/6-31G*

E(RB-P86) = -519.527335985

Zero-point correction= 0.234056 (Hartree/Particle)

Thermal correction to Energy= 0.247167

Thermal correction to Enthalpy= 0.248111

Thermal correction to Gibbs Free Energy= 0.194269

Sum of electronic and zero-point Energies= -519.293280

Sum of electronic and thermal Energies= -519.280169

Sum of electronic and thermal Enthalpies= -519.279225

Sum of electronic and thermal Free Energies= -519.333067

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	155.099	48.247	113.319

C,0,2.0129905536,-0.806028919,-2.2561888253

O,0,2.7719166871,0.4355540545,-2.3902539509

C,0,2.7869913935,0.9630266253,-3.6230404905

O,0,2.2251143039,0.495005513,-4.6066354132

C,0,3.6283368292,2.242270385,-3.57255966

N,0,3.7202529208,2.9942640214,-4.8801700265

C,0,4.4386938758,2.170663897,-5.9237452049

C,0,4.5151158136,4.2512866147,-4.6155888788

C,0,2.3235901342,3.3861862608,-5.4308281665

C,0,1.4664325839,4.0684916027,-4.4060942262

C,0,1.228062736,5.3916569398,-4.4293259876

H,0,2.1194820968,-1.0897703338,-1.2004945906

H,0,0.957584927,-0.6247156969,-2.5167140087

H,0,2.4385992842,-1.5743627328,-2.9218522211

H,0,4.6584255489,1.993723304,-3.2683764725

H,0,3.2066185688,2.9319763466,-2.823487024

H,0,3.8577635518,1.2550263589,-6.0951921259

H,0,4.502871181,2.7744993353,-6.8413115718

H,0,5.4448379724,1.9402449393,-5.5420096337

H,0,5.4940690489,3.960945586,-4.20618961

H,0,4.6365627206,4.7811093272,-5.5718257214

H,0,3.9532081674,4.8695144853,-3.9002772688

H,0,2.5394161728,4.0405015702,-6.29045421

H,0,1.8806807854,2.4405551591,-5.7760013263

H,0,0.9996498195,3.4333242234,-3.6427493112

H,0,1.669481779,6.0363327894,-5.2000458559

H,0,0.5722825436,5.8660363434,-3.6909112178

TS/ BP86GD2 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSBP86PCMSBGD2

parent ts exo s-cis

BP86/6-31G*

E(RB-P86) = -519.021844990

Zero-point correction= 0.216846 (Hartree/Particle)

Thermal correction to Energy= 0.229709

Thermal correction to Enthalpy= 0.230654

Thermal correction to Gibbs Free Energy= 0.178653

Sum of electronic and ZPE= -518.804999

Sum of electronic and thermal Energies= -518.792136

Sum of electronic and thermal Enthalpies= -518.791191

Sum of electronic and thermal Free Energies= -518.843192

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	144.145	48.034	109.444

C,0,1.9754168932,-0.8287999233,-2.3896795892

O,0,2.7444856205,0.3872940752,-2.460900231

C,0,2.812249073,0.9426429397,-3.7330465669

C,0,3.5156023018,2.1868405879,-3.6994277285

N,0,3.8275202427,2.8914014679,-4.8583465692

C,0,4.6459095506,4.0935191662,-4.5810051569

O,0,2.2840747728,0.3857386765,-4.719454277

C,0,4.3524016962,2.1248609761,-6.0164767917

C,0,2.1171535783,3.7308245898,-5.6860392088

C,0,1.5235395408,4.2488648424,-4.5080504564

C,0,1.0206275209,3.380247323,-3.5655340074

H,0,2.0201405897,-1.1435684968,-1.3351005414

H,0,0.926868126,-0.65404666,-2.6937525229

H,0,2.4055172225,-1.6098942261,-3.0428029366

H,0,3.7819111106,2.6440711292,-2.7473285633

H,0,5.3872700556,1.8001740933,-5.7998035648

H,0,3.7015084627,1.2540448151,-6.1753800253

H,0,4.3416928937,2.7850458204,-6.8996566006

H,0,5.6285179205,3.7898993472,-4.1745265781

H,0,4.7804133195,4.6554155539,-5.5186165897

H,0,4.1086768849,4.7154353583,-3.8468823187

H,0,2.5430688353,4.3982962648,-6.4448719029

H,0,1.7828603409,2.7482993869,-6.0425752275

H,0,1.7039321495,5.2992945108,-4.2406721573

H,0,0.7659427832,2.3532684604,-3.8464828173

H,0,0.716952515,3.7182909213,-2.5676270706

Cation/ B3LYPGD3/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2B3LYPPCMSBGD3

parent sm conf 2

B3LYP/6-31G*

E(RB3LYP) = -519.528552243

Zero-point correction= 0.242322 (Hartree/Particle)

Thermal correction to Energy= 0.255129

Thermal correction to Enthalpy= 0.256073

Thermal correction to Gibbs Free Energy= 0.202846

Sum of electronic and zero-point Energies= -519.286230

Sum of electronic and thermal Energies= -519.273424

Sum of electronic and thermal Enthalpies= -519.272479

Sum of electronic and thermal Free Energies= -519.325707

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	160.096	46.797	112.026

C,0,2.0071022247,-0.776382545,-2.2475641334

O,0,2.7802617735,0.4411707824,-2.4058465496

C,0,2.7742781201,0.9846673246,-3.6182711913

O,0,2.1806066683,0.5486663872,-4.5834078193

C,0,3.6346685899,2.2432126723,-3.580670352

N,0,3.7327104093,2.9960608849,-4.8850859586

C,0,4.4452722385,2.1643409319,-5.9261205285

C,0,4.542001335,4.2433046725,-4.6189665001

C,0,2.3449951647,3.4041037702,-5.4437368399

C,0,1.4528567462,4.0418596774,-4.4235802743

C,0,1.1866528596,5.3495416847,-4.4041314277

H,0,2.1371008719,-1.0628610283,-1.2056387024

H,0,0.9562389812,-0.5801931479,-2.4700287023

H,0,2.3912060882,-1.5498577025,-2.9157644363

H,0,4.6483949695,1.9699710437,-3.2792859015

H,0,3.2375178935,2.9240817428,-2.8258318497

H,0,3.8797028422,1.249798288,-6.088345609

H,0,4.5027212983,2.7452367188,-6.8467608867

H,0,5.4482776864,1.939233658,-5.5624424167

H,0,5.5056327465,3.9536496221,-4.200082511

H,0,4.6862994476,4.7680091573,-5.563066279

H,0,3.9946986569,4.8734377724,-3.9190156756

H,0,2.5639035617,4.0811513476,-6.271052845

H,0,1.9093421741,2.4852578897,-5.8322729478

H,0,0.9740357179,3.3778611461,-3.7070491127

H,0,1.6294457915,6.0358152895,-5.1222779496

H,0,0.5031071424,5.7761799596,-3.6760256004

TS/ B3LYPGD3 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSB3LYPPCMSBGD3

parent ts exo s-cis

B3LYP/6-31G*

E(RB3LYP) = -519.011856695

Zero-point correction= 0.224523 (Hartree/Particle)

Thermal correction to Energy= 0.237051

Thermal correction to Enthalpy= 0.237995

Thermal correction to Gibbs Free Energy= 0.186593

Sum of electronic and ZPE= -518.787334

Sum of electronic and thermal Energies= -518.774806

Sum of electronic and thermal Enthalpies= -518.773862

Sum of electronic and thermal Free Energies= -518.825264

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.752	46.541	108.185

C,0,1.9866846467,-0.8015225046,-2.3669378769

O,0,2.7412570102,0.4094627254,-2.4690339087

C,0,2.8184042089,0.9479447164,-3.733921268

C,0,3.5093184178,2.1909031702,-3.7129085486

N,0,3.8327248315,2.8918089264,-4.8632179052

C,0,4.6762030536,4.0716894223,-4.5806906754

O,0,2.3063549903,0.3764456728,-4.7071852919

C,0,4.340996961,2.1233313228,-6.0232718209

C,0,2.1097103892,3.7729455719,-5.6829787854

C,0,1.5023653673,4.2286754139,-4.4950232621

C,0,0.9896523656,3.3364742385,-3.5949018789

H,0,2.0283818312,-1.0883825688,-1.3146522924

H,0,0.9459704744,-0.6473413973,-2.6713209823

H,0,2.4186206923,-1.592630499,-2.9883025513

H,0,3.7795834301,2.6337124602,-2.7663263314

H,0,5.3567282935,1.7706865553,-5.8101993241

H,0,3.6843765219,1.2750298114,-6.1994126786

H,0,4.3564293874,2.7771783264,-6.8980707305

H,0,5.6466770861,3.751462259,-4.1848400888

H,0,4.8244975744,4.6381499319,-5.5011846436

H,0,4.1708338851,4.701099242,-3.8461222957

H,0,2.5241815033,4.4775310782,-6.3990899215

H,0,1.7860123278,2.8225622243,-6.0974880062

H,0,1.669824969,5.2605525083,-4.187904618

H,0,0.7359750628,2.3262885636,-3.8971618144

H,0,0.6724887185,3.6434038287,-2.6018924991

Cation/ M06GD3/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2M06PCMSBGD3

parent sm conf 2

M06/6-31G*

E(RM06) = -519.153693058

Zero-point correction= 0.240263 (Hartree/Particle)

Thermal correction to Energy= 0.253066

Thermal correction to Enthalpy= 0.254010

Thermal correction to Gibbs Free Energy= 0.200939

Sum of electronic and zero-point Energies= -518.913430

Sum of electronic and thermal Energies= -518.900627

Sum of electronic and thermal Enthalpies= -518.899683

Sum of electronic and thermal Free Energies= -518.952754

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	158.801	47.046	111.697

C,0,2.0455191788,-0.7824688665,-2.2736836244

O,0,2.8073855096,0.42681895,-2.4187059667

C,0,2.7747204393,0.9886404351,-3.6148319811

O,0,2.168559344,0.5672155385,-4.5724415938

C,0,3.6171754479,2.2453239062,-3.5718128528

N,0,3.7127282613,2.9906642058,-4.8665914065 C,0,4.4189825183,2.1622443883,-5.8980702741

C,0,4.5230869859,4.2240403233,-4.6070984084 C,0,2.3402975794,3.400326728,-5.4256402855

C,0,1.4626331018,4.0632222767,-4.4227185167

C,0,1.2074696891,5.36933152,-4.4458473339

H,0,2.2094918964,-1.1120002763,-1.2481534726

H,0,0.9855772451,-0.5784108837,-2.4489664623

H,0,2.3994048548,-1.5360000816,-2.9826074863

H,0,4.6371898701,1.9849602238,-3.2653138959

H,0,3.21611523,2.9257730238,-2.8120154249

H,0,3.8479374067,1.2478689885,-6.0671930803

H,0,4.4846065527,2.7465184995,-6.8194146989

H,0,5.4220543397,1.9306463218,-5.5303997

H,0,5.4939969952,3.9288503504,-4.2016562129

H,0,4.6567777862,4.7541615228,-5.5532691794

H,0,3.9905912044,4.8567794985,-3.8931543976

H,0,2.569063657,4.0649322424,-6.2662148639

H,0,1.8950465333,2.4783911678,-5.8077106484

H,0,0.9758274121,3.4224964663,-3.6852909445

H,0,1.6576477382,6.0259985625,-5.1910343292

H,0,0.5291452224,5.8309929679,-3.7324859592

TS/ M06GD3 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSM06PCMSBGD3

parent ts exo s-cis

M06/6-31G*

E(RM06) = -518.636532007

Zero-point correction= 0.222776 (Hartree/Particle)

Thermal correction to Energy= 0.235400

Thermal correction to Enthalpy= 0.236344

Thermal correction to Gibbs Free Energy= 0.184630

Sum of electronic and ZPE= -518.413756

Sum of electronic and thermal Energies= -518.401132

Sum of electronic and thermal Enthalpies= -518.400188

Sum of electronic and thermal Free Energies= -518.451902

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.716	46.776	108.841

C,0,1.9687402095,-0.735901955,-2.3381080529

O,0,2.714598796,0.4622698015,-2.4611407738

C,0,2.8329816531,0.9417399961,-3.7348623201

C,0,3.4646191692,2.2169739513,-3.7266952061

N,0,3.8125749001,2.900102372,-4.8747522137

C,0,4.6731788603,4.0531098462,-4.5916999336

O,0,2.3915643397,0.3141327407,-4.6971365788

C,0,4.3085005006,2.1326811389,-6.0257958101

C,0,2.1128160148,3.8288892221,-5.6801159045

C,0,1.5094433467,4.1984372726,-4.4735282658

C,0,1.0581723224,3.2211798605,-3.6295642329

H,0,1.9791593152,-0.993009333,-1.2762334932

H,0,0.9341564602,-0.5933982801,-2.6754117842

H,0,2.4152043352,-1.5492123669,-2.9217322006

H,0,3.7328953931,2.6672546987,-2.7774234389

H,0,5.3247568828,1.7694451398,-5.8184397591

H,0,3.6449777128,1.2859662781,-6.2034643039

H,0,4.3294912044,2.7896224806,-6.9022218347

H,0,5.6417745378,3.7117941402,-4.2011399737

H,0,4.8310802808,4.6247860416,-5.5114934659

H,0,4.1865982861,4.6916022487,-3.8474214218

H,0,2.5364684089,4.5746832519,-6.3533675377

H,0,1.7994976012,2.8993972573,-6.1576335792

H,0,1.6727258168,5.207986358,-4.0899348123

H,0,0.7822745821,2.2425844388,-4.0191668983

H,0,0.7560030703,3.4343443996,-2.6055562038

Cation/ PBE0GD3/6-31G*/PCM- Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2PBE0PCMSBGD3

parent sm conf 2

PBE1PBE/6-31G*

E(RPBE1PBE) = -518.911312025

Zero-point correction= 0.243794 (Hartree/Particle)

Thermal correction to Energy= 0.256526

Thermal correction to Enthalpy= 0.257470

Thermal correction to Gibbs Free Energy= 0.204542

Sum of electronic and zero-point Energies= -518.667518

Sum of electronic and thermal Energies= -518.654786

Sum of electronic and thermal Enthalpies= -518.653842

Sum of electronic and thermal Free Energies= -518.706770

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	160.973	46.479	111.396

C,0,2.0149126296,-0.7571899549,-2.2693600272

O,0,2.7748845503,0.4544501958,-2.4141465477

C,0,2.7851715512,0.9853049554,-3.6241313143

O,0,2.2127928843,0.537146961,-4.5917018791

C,0,3.6329359825,2.2431200121,-3.5851480135

N,0,3.723870322,2.9906532391,-4.8772207773

C,0,4.4289794016,2.1708848288,-5.9129734682

C,0,4.5232590544,4.2281786666,-4.6138584148

C,0,2.3494474189,3.3892224325,-5.4213729963

C,0,1.4740771538,4.04545354,-4.4059825894

C,0,1.2013316902,5.3496665706,-4.4203695351

H,0,2.1274446644,-1.0450305099,-1.2259206501

H,0,0.9659317829,-0.5709054368,-2.5083407315

H,0,2.4136620937,-1.5301240991,-2.9294026408

H,0,4.6490407198,1.975107461,-3.2835754566

H,0,3.2340155873,2.9207670669,-2.8265381284

H,0,3.8621814612,1.2575101128,-6.082375925

H,0,4.4892912386,2.756151265,-6.8312101203

H,0,5.4320759099,1.940923676,-5.551514414

H,0,5.492259521,3.9413269242,-4.2044739181

H,0,4.65872052,4.7594030474,-5.556175536

H,0,3.9805983573,4.854550903,-3.9057952823

H,0,2.5578615842,4.0543372328,-6.2622183824

H,0,1.9028656939,2.4668609995,-5.7936039045

H,0,1.0046842248,3.4008056386,-3.6650371633

H,0,1.6307845071,6.0159734013,-5.1653251848

H,0,0.5259514949,5.7927688702,-3.694549999

TS/ PBE0GD3 /6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSPBE0PCMSBGD3

parent ts exo s-cis

PBE1PBE/6-31G*

E(RPBE1PBE) = -518.392479456

Zero-point correction= 0.226405 (Hartree/Particle)

Thermal correction to Energy= 0.238737

Thermal correction to Enthalpy= 0.239681

Thermal correction to Gibbs Free Energy= 0.188764

Sum of electronic and ZPE= -518.166074

Sum of electronic and thermal Energies= -518.153743

Sum of electronic and thermal Enthalpies= -518.152798

Sum of electronic and thermal Free Energies= -518.203716

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.810	45.920	107.164

C,0,2.0145562325,-0.7913118165,-2.3718084097

O,0,2.7201242151,0.4366837062,-2.4733323536

C,0,2.7859948012,0.9602679804,-3.7320044668

C,0,3.4143454864,2.2353887925,-3.7168002437

N,0,3.7767889675,2.9076773035,-4.8716482687

C,0,4.6412266428,4.0569340951,-4.5794916535

O,0,2.3019165306,0.3648549915,-4.6981191734

C,0,4.2965082005,2.1170355324,-5.9972030348

C,0,2.145150778,3.7958460254,-5.6853552582

C,0,1.5291806279,4.2427954714,-4.5044461232

C,0,1.0782328154,3.3030529032,-3.616947438

H,0,2.0523749073,-1.069998597,-1.3175457629

H,0,0.9731137467,-0.6785222755,-2.6899556748

H,0,2.4828549078,-1.5707792471,-2.9807683046

H,0,3.725397308,2.6615117889,-2.7739769182

H,0,5.3046103198,1.7582984097,-5.7612081474

H,0,3.6343503049,1.2708923894,-6.1695072577

H,0,4.3347640207,2.7540485966,-6.8843872894

H,0,5.5904103039,3.712579564,-4.1541860229

H,0,4.8317781845,4.6104475493,-5.5008131647

H,0,4.1355137299,4.7082263123,-3.8637194482

H,0,2.5703765824,4.5032628788,-6.3946348841

H,0,1.798939724,2.8610411401,-6.1220599752

H,0,1.7099087689,5.2625772103,-4.1669415955

H,0,0.7760514863,2.319991988,-3.9653567153

H,0,0.7897844072,3.5646583073,-2.6018224152

Cation/ B3LYP /6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/Parentcalcs/SM2B3LYPPSPCMSB

parent sm conf 2

B3LYP/6-31G*

E(RB3LYP) = -519.501174619

Zero-point correction= 0.241778 (Hartree/Particle)

Thermal correction to Energy= 0.254736

Thermal correction to Enthalpy= 0.255680

Thermal correction to Gibbs Free Energy= 0.202048

Sum of electronic and ZPE= -519.259397

Sum of electronic and thermal Energies= -519.246439

Sum of electronic and thermal Enthalpies= -519.245495

Sum of electronic and thermal Free Energies= -519.299126

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.849	47.134	112.878

C,0,2.057310332,-0.8525210663,-2.2644215254

O,0,2.8004239017,0.3836051209,-2.4133833706

C,0,2.7811731767,0.9430577525,-3.618858864

O,0,2.196147222,0.5059513815,-4.5887552883

C,0,3.6175854908,2.2194814405,-3.5641303376

N,0,3.7125583763,2.9930236554,-4.8571188975

C,0,4.4128834307,2.1733844154,-5.9158875469

C,0,4.5368527192,4.227047812,-4.5795129339

C,0,2.3249993452,3.4161127604,-5.3999901168

C,0,1.4775098647,4.1532393317,-4.4079726935

C,0,1.1854150316,5.4507017515,-4.523475005

H,0,2.1946047229,-1.1423502822,-1.2244671487

H,0,1.0021190179,-0.6807220039,-2.4841088156

H,0,2.461033324,-1.6120347478,-2.9362773631

H,0,4.6352669684,1.9608902164,-3.2626365805

H,0,3.2078664526,2.8848422748,-2.8020791317

H,0,3.8269071757,1.2778770232,-6.1076533313

H,0,4.4940904395,2.7791455699,-6.8183711727

H,0,5.4068489108,1.9140964916,-5.5500692251

H,0,5.5063919083,3.9194221315,-4.1880586108

H,0,4.6657064237,4.7713277048,-5.514880347

H,0,4.0113098307,4.8465578523,-3.8544571307

H,0,2.5412489232,4.0317356399,-6.2744482588

H,0,1.8510950239,2.4882231086,-5.7190619141

H,0,1.0351231637,3.5703576534,-3.6027360935

H,0,1.5847069846,6.0610956377,-5.3302437229

H,0,0.5218538388,5.9437693743,-3.8192675742

TS/ B3LYP/6-31G*/PCM

/home/bibaswanbiswas/c8/Parentcalcs/TSB3LYPPSPCMSB

parent ts exo s-cis

B3LYP/6-31G*

E(RB3LYP) = -518.984732518

Zero-point correction= 0.224070 (Hartree/Particle)

Thermal correction to Energy= 0.236778

Thermal correction to Enthalpy= 0.237722

Thermal correction to Gibbs Free Energy= 0.185859

Sum of electronic and ZPE= -518.760663

Sum of electronic and thermal Energies= -518.747955

Sum of electronic and thermal Enthalpies= -518.747011

Sum of electronic and thermal Free Energies= -518.798874

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 148.580 46.847 109.155

C,0,2.036326266,-0.8273470306,-2.3371917288

O,0,2.7383275449,0.4126488013,-2.4535910539

C,0,2.8112976155,0.9339679026,-3.7268721839

C,0,3.4742243681,2.1939486613,-3.7153756902

N,0,3.8161979518,2.8917848668,-4.8627768863

C,0,4.6993609501,4.0414038579,-4.5735449359

O,0,2.3271350897,0.3295760773,-4.693978429

C,0,4.3050334079,2.1132864994,-6.02497574

C,0,2.1287052447,3.8367035771,-5.6875491085

C,0,1.4944377057,4.2670291683,-4.5032165916

C,0,0.9404699723,3.3611140797,-3.6436048471

H,0,2.0819040609,-1.0938451002,-1.2798134553

H,0,0.9924168064,-0.724546189,-2.6505133129

H,0,2.5080435058,-1.6094425911,-2.9400318655

H,0,3.7370555229,2.6429043213,-2.769327603

H,0,5.3129187747,1.7369086231,-5.8141777511

H,0,3.6299157112,1.2787320813,-6.1978464715

H,0,4.3362921509,2.7678431748,-6.8986918264

H,0,5.6612609436,3.6853948294,-4.1873131794

H,0,4.8615948605,4.6115290266,-5.4893981531

H,0,4.2220427584,4.6794049961,-3.8279856004

H,0,2.5661072001,4.5590549983,-6.3718244395

H,0,1.7924817197,2.9113322098,-6.1460772055

H,0,1.6589167755,5.2901196078,-4.1661107056

H,0,0.6938230932,2.3582881637,-3.9754079135

H,0,0.5879639995,3.6496663871,-2.6568433221

Cation/M11/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2M11

parent sm conf 2

M11/6-31G*

E(RM11) = -519.215307678

Zero-point correction= 0.241865 (Hartree/Particle)

Thermal correction to Energy= 0.254549

Thermal correction to Enthalpy= 0.255493

Thermal correction to Gibbs Free Energy= 0.202879

Sum of electronic and ZPE= -518.973442

Sum of electronic and thermal Energies= -518.960759

Sum of electronic and thermal Enthalpies= -518.959814

Sum of electronic and thermal Free Energies= -519.012428

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 159.732 46.564 110.735

C,0,2.013806569,-0.7434856016,-2.2705517241

O,0,2.7993331706,0.4596143627,-2.4088108433

C,0,2.7645167358,1.032736886,-3.5991101612

O,0,2.1346744659,0.6217342909,-4.548558019

C,0,3.6261132855,2.2867533376,-3.5757093088

N,0,3.7248902429,2.994888796,-4.8903262262

C,0,4.4412938844,2.1437312634,-5.8964992964

C,0,4.5228935216,4.2430065377,-4.651455869

C,0,2.3597294168,3.3845848485,-5.4649368007

C,0,1.4471026475,3.9820840322,-4.4333738678

C,0,1.2233994629,5.2913174387,-4.3491196041

H,0,2.1525431586,-1.0683316058,-1.237246996

H,0,0.9605051198,-0.5203671706,-2.4742769724

H,0,2.3777177804,-1.5017713835,-2.972910936

H,0,4.6419490586,2.0166956705,-3.2605357112

H,0,3.2172728579,2.9872328449,-2.8360616535

H,0,3.8754340011,1.2192683976,-6.0383814519

H,0,4.499446002,2.7033408263,-6.8362188558

H,0,5.4485944109,1.9323823316,-5.5215326827

H,0,5.4890086446,3.9657715371,-4.2168489018

H,0,4.6725463785,4.7476631077,-5.6115371164

H,0,3.9646820028,4.8880366093,-3.9648344073

H,0,2.5800950538,4.0987240646,-6.2678561992

H,0,1.9385594964,2.4708745975,-5.8929686747

H,0,0.9258220151,3.2891474507,-3.7673407634

H,0,1.7123163756,5.9983318894,-5.0246124749

H,0,0.5347862408,5.7033526405,-3.6107074824

TS M11 /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentRM11

parent ts exo s-cis

M11/6-31G*

E(RM11) = -518.690990016

Zero-point correction= 0.225201 (Hartree/Particle)

Thermal correction to Energy= 0.237309

Thermal correction to Enthalpy= 0.238253

Thermal correction to Gibbs Free Energy= 0.187899

Sum of electronic and ZPE= -518.465789

Sum of electronic and thermal Energies= -518.453681

Sum of electronic and thermal Enthalpies= -518.452737

Sum of electronic and thermal Free Energies= -518.503091

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.914	45.420	105.979

C,0,1.9990917477,-0.8112708507,-2.4148524687

O,0,2.7001513553,0.4302106947,-2.4859167187

C,0,2.7495685992,0.993033897,-3.7243880246

C,0,3.3430589892,2.2914997784,-3.6957182915

N,0,3.7370903755,2.925646042,-4.8752369696

C,0,4.5914363378,4.0892728446,-4.5839555614

O,0,2.2389276698,0.4314893392,-4.6965288329

C,0,4.304068565,2.110158674,-5.9670670415

C,0,2.1506683135,3.7345696062,-5.6833049862

C,0,1.5461271804,4.2530791161,-4.5250848203

C,0,1.2116856179,3.304505757,-3.5820433471

H,0,2.0324822657,-1.119247934,-1.365125744

H,0,0.9581539807,-0.6883524325,-2.7420112782

H,0,2.4821726422,-1.5668193404,-3.0480770708

H,0,3.7613038927,2.65800439,-2.7636197539

H,0,5.3143666309,1.7742682083,-5.6932017149

H,0,3.655136416,1.249791411,-6.1426587714

H,0,4.3590426437,2.7334071112,-6.8693983809

H,0,5.5369242546,3.7537462161,-4.1344128266

H,0,4.7948015714,4.6315184871,-5.5151569955

H,0,4.0611508985,4.7441266682,-3.8823751498

H,0,2.5620728306,4.3967247893,-6.4517186358

H,0,1.7830493066,2.7732873481,-6.0603788629

H,0,1.743098458,5.2857706078,-4.2278544805

H,0,0.8218071774,2.3397580505,-3.9132593075

H,0,0.9768162801,3.5792825208,-2.5506939644

Cation/M11L/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2M11L

parent sm conf 2

M11L/6-31G*

E(RM11L) = -519.327287478

Zero-point correction= 0.236445 (Hartree/Particle)

Thermal correction to Energy= 0.249534

Thermal correction to Enthalpy= 0.250478

Thermal correction to Gibbs Free Energy= 0.196184

Sum of electronic and ZPE= -519.090842

Sum of electronic and thermal Energies= -519.077754

Sum of electronic and thermal Enthalpies= -519.076809

Sum of electronic and thermal Free Energies= -519.131103

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	156.585	47.456	114.271

C,0,2.0340726827,-0.7141607078,-2.2956807733

O,0,2.7975032983,0.4751438145,-2.4216748932

C,0,2.7789965695,1.0081121502,-3.613020059

O,0,2.1871339235,0.5800854356,-4.5592651837

C,0,3.6262127796,2.2555072033,-3.5833596618

N,0,3.7158436265,2.979869074,-4.8698050726

C,0,4.4092253537,2.1645056277,-5.8883078243

C,0,4.5124352099,4.1991356037,-4.6181554417

C,0,2.363157209,3.3829515876,-5.4171054596

C,0,1.4793288015,4.0166038477,-4.4101481697

C,0,1.2056823388,5.3141635285,-4.4100191268

H,0,2.1714024365,-1.0385321175,-1.2592295894

H,0,0.9735114883,-0.5084838496,-2.4988183743

H,0,2.4027966811,-1.4801262934,-2.9922017889

H,0,4.6504699593,1.9938725382,-3.2736468666

H,0,3.2342121104,2.9502944273,-2.8234833588

H,0,3.8348356963,1.2502436169,-6.0751540558

H,0,4.4834926659,2.7536043489,-6.8117514936

H,0,5.416091875,1.9194670255,-5.5256989758

H,0,5.4897379563,3.9118707302,-4.2093409584

H,0,4.6490877471,4.733725536,-5.5669352691

H,0,3.978894462,4.8381307623,-3.9022942272

H,0,2.5875306608,4.0710919679,-6.2481830219

H,0,1.920389963,2.4656868419,-5.8310136926

H,0,0.9848582509,3.3561711575,-3.6851868708

H,0,1.6520761694,5.996229451,-5.1439171394

H,0,0.510052084,5.7521546916,-3.688925652

TS/ M11L /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentM11L

parent ts exo s-cis

M11L/6-31G*

E(RM11L) = -518.821863825

Zero-point correction= 0.219343 (Hartree/Particle)

Thermal correction to Energy= 0.232208

Thermal correction to Enthalpy= 0.233152

Thermal correction to Gibbs Free Energy= 0.180989

Sum of electronic and ZPE= -518.602521

Sum of electronic and thermal Energies= -518.589656

Sum of electronic and thermal Enthalpies= -518.588712

Sum of electronic and thermal Free Energies= -518.640875

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	145.713	47.624	109.786

C,0,2.0095406451,-0.72564397,-2.3735716423

O,0,2.731754584,0.4662964057,-2.4699275684

C,0,2.8367125147,0.9396694693,-3.727091124

C,0,3.5210538354,2.1825241292,-3.7206445947

N,0,3.8350356761,2.8686153217,-4.8491774867

C,0,4.6679071403,4.0188828505,-4.5812113521

O,0,2.37709327,0.33050037,-4.6735954095

C,0,4.2982578508,2.1249668546,-6.0027468325

C,0,2.116740734,3.8101927789,-5.6776950658

C,0,1.5206337475,4.2028141153,-4.4784315519

C,0,0.9955289859,3.282645183,-3.62800938

H,0,2.0163858236,-0.9981143903,-1.3097786909

H,0,0.9691545833,-0.5968832365,-2.7177991351

H,0,2.4719401923,-1.5316791614,-2.9668747524

H,0,3.7171352259,2.6753565977,-2.7697082489

H,0,5.3166917913,1.7377680333,-5.8161416154

H,0,3.6215786873,1.2865124428,-6.1999039035

H,0,4.3233798739,2.8003556143,-6.8711198931

H,0,5.6547037726,3.6999271946,-4.1995566528

H,0,4.8067942001,4.5980744093,-5.5049976716

H,0,4.1803589147,4.654721741,-3.8272146509

H,0,2.5369292548,4.5499492148,-6.3692604597

H,0,1.7933034264,2.8679295877,-6.1387058921

H,0,1.6995887121,5.2250808643,-4.1139468787

H,0,0.7343641301,2.2812458317,-3.9880619001

H,0,0.6616864279,3.5457527485,-2.6188676466

Cation/MN12L/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2MN12L

parent sm conf 2

MN12L/6-31G*

E(RMN12L) = -518.951419795

Zero-point correction= 0.243871 (Hartree/Particle)

Thermal correction to Energy= 0.256423

Thermal correction to Enthalpy= 0.257367

Thermal correction to Gibbs Free Energy= 0.205228

Sum of electronic and ZPE= -518.707549

Sum of electronic and thermal Energies= -518.694997

Sum of electronic and thermal Enthalpies= -518.694053

Sum of electronic and thermal Free Energies= -518.746192

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.908	46.170	109.736

C,0,2.0169828434,-0.7049087757,-2.2646252304

O,0,2.8214020853,0.4688281021,-2.421525019

C,0,2.7473463566,1.0593237716,-3.5941676346

O,0,2.0742201311,0.6835027372,-4.5237617892

C,0,3.6215110641,2.292299404,-3.5805403752

N,0,3.7304764188,2.9893785149,-4.8974695711

C,0,4.4439388277,2.1340062105,-5.8924629489

C,0,4.5354299227,4.226101261,-4.6561476084

C,0,2.375961661,3.4023031116,-5.4890249093

C,0,1.4405066955,3.9377820435,-4.4578548506

C,0,1.1979407051,5.23852889,-4.3143488262

H,0,2.2028163389,-1.0523615892,-1.2497499573

H,0,0.9619720487,-0.4545475411,-2.4031232884

H,0,2.315630011,-1.461045135,-2.9952848126

H,0,4.6348888965,2.023795922,-3.2613690998

H,0,3.2274952561,3.0085075336,-2.848846377

H,0,3.8792340087,1.2114559982,-6.0344115308

H,0,4.5054567972,2.6860273103,-6.8337363302

H,0,5.4484894764,1.9222221105,-5.5175272614

H,0,5.4863332028,3.9455736066,-4.1967145379

H,0,4.7129607197,4.7183498625,-5.6149824195

H,0,3.9712686967,4.8848383834,-3.9899332592

H,0,2.621360098,4.1562353184,-6.2457295124

H,0,1.9767818243,2.5120784534,-5.9800775181

H,0,0.9201506744,3.2043932581,-3.8386948965

H,0,1.6868017534,5.9832118681,-4.9439749433

H,0,0.4916754857,5.6114373694,-3.5762384927

TS MN12L /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentMN12L

parent ts exo s-cis

MN12L/6-31G*

E(RMN12L) = -518.439201710

Zero-point correction= 0.224956 (Hartree/Particle)

Thermal correction to Energy= 0.237571

Thermal correction to Enthalpy= 0.238515

Thermal correction to Gibbs Free Energy= 0.187105

Sum of electronic and ZPE= -518.214246

Sum of electronic and thermal Energies= -518.201631

Sum of electronic and thermal Enthalpies= -518.200687

Sum of electronic and thermal Free Energies= -518.252097

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.078	46.711	108.202

C,0,1.9325265401,-0.7508724864,-2.4177255391

O,0,2.7170502308,0.4228731216,-2.4924549408

C,0,2.8277003282,0.9613161688,-3.7321307835

C,0,3.5506798141,2.1827082858,-3.6992814757

N,0,3.8753187468,2.8671519167,-4.8406527571

C,0,4.6383874729,4.0820319173,-4.5779163876

O,0,2.3142950986,0.4212165155,-4.7118213978

C,0,4.3704887247,2.1363986189,-6.0074113063

C,0,2.0513133216,3.7074753426,-5.694436471

C,0,1.5301949616,4.1859552394,-4.4927277437

C,0,1.0772902443,3.3116195317,-3.5408447492

H,0,1.9336110014,-1.046796882,-1.3671227755

H,0,0.9059275494,-0.561921754,-2.7528625601

H,0,2.357600805,-1.5512155504,-3.0338360351

H,0,3.8113550426,2.634157997,-2.749150699

H,0,5.4026389585,1.8015658996,-5.8283307079

H,0,3.7303831307,1.2747687489,-6.198188285

H,0,4.3565031475,2.8115284725,-6.8700028638

H,0,5.6393024901,3.8330449033,-4.1965601213

H,0,4.7343930399,4.6573539976,-5.5034037427

H,0,4.1058646098,4.6799040948,-3.8309618009

H,0,2.4541346334,4.3739779979,-6.4564170948

H,0,1.7835271296,2.7014370055,-6.022651614

H,0,1.705070261,5.2299114483,-4.2228516363

H,0,0.7947015077,2.297662185,-3.8189691612

H,0,0.8139952099,3.6342082642,-2.5353273505

Cation/MN12SX/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2MN12SX

parent sm conf 2

MN12SX/6-31G*

E(RMN12SX) = -519.055212320

Zero-point correction= 0.243315 (Hartree/Particle)

Thermal correction to Energy= 0.256065

Thermal correction to Enthalpy= 0.257009

Thermal correction to Gibbs Free Energy= 0.203999

Sum of electronic and ZPE= -518.811897

Sum of electronic and thermal Energies= -518.799148

Sum of electronic and thermal Enthalpies= -518.798203

Sum of electronic and thermal Free Energies= -518.851213

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.683	46.526	111.568

C,0,2.0281694498,-0.7407991288,-2.2597276378

O,0,2.8045796994,0.4532522075,-2.4152862507

C,0,2.7613065696,1.0185275437,-3.6058803058

O,0,2.1298370753,0.6081280331,-4.55095102

C,0,3.6201832717,2.2684272683,-3.582887212

N,0,3.7223891657,2.9896468148,-4.8883232399

C,0,4.4333645787,2.1518370637,-5.9040637475

C,0,4.5304091009,4.2239768983,-4.6334600956

C,0,2.3627073007,3.4013170035,-5.4604974291

C,0,1.4487959128,3.9987531627,-4.4400784115

C,0,1.2034057908,5.3045625773,-4.3689791727

H,0,2.1781859981,-1.0535024724,-1.2247177199

H,0,0.9708519164,-0.5281763601,-2.4511840208

H,0,2.3831491218,-1.5113184309,-2.9526235966

H,0,4.6364182629,1.9997729765,-3.2674002712

H,0,3.21887838,2.9648759309,-2.8351381606

H,0,3.8613161089,1.2371373718,-6.0759034449

H,0,4.5092105174,2.7284893397,-6.8311637816

H,0,5.4344609597,1.9181770637,-5.5285291764

H,0,5.4960734437,3.9340197119,-4.2083652411

H,0,4.6815417218,4.7444494503,-5.5836470014

H,0,3.9858448762,4.8655335844,-3.9338950254

H,0,2.5962554744,4.1161178581,-6.2590217599

H,0,1.9342173749,2.4973665256,-5.9040192549

H,0,0.9324569263,3.3065492853,-3.7702438898

H,0,1.6815144361,6.0164458883,-5.0452024419

H,0,0.5035085656,5.7137508328,-3.6411336914

TS MN12SX /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentMN12SX

parent ts exo s-cis

MN12SX/6-31G*

E(RMN12SX) = -518.540322510

Zero-point correction= 0.225346 (Hartree/Particle)

Thermal correction to Energy= 0.237939

Thermal correction to Enthalpy= 0.238883

Thermal correction to Gibbs Free Energy= 0.187252

Sum of electronic and ZPE= -518.314977

Sum of electronic and thermal Energies= -518.302383

Sum of electronic and thermal Enthalpies= -518.301439

Sum of electronic and thermal Free Energies= -518.353071

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.309	46.521	108.668

C,0,1.9797597537,-0.7607466632,-2.3636653209

O,0,2.7068764343,0.4484683514,-2.4699473142

C,0,2.8065465414,0.9550897391,-3.729179851

C,0,3.4687007415,2.2132052718,-3.7179805179

N,0,3.8202691512,2.8885693683,-4.8642165818

C,0,4.6537565714,4.058653194,-4.5825581064

O,0,2.3273241175,0.3579310035,-4.6941428454

C,0,4.3195655022,2.1282363583,-6.0151205034

C,0,2.1035482905,3.7958027652,-5.6914997539

C,0,1.5254505726,4.2113985371,-4.4877797194

C,0,1.0700142336,3.2691759675,-3.6060422852

H,0,1.991149565,-1.026584899,-1.3023718482

H,0,0.9439217018,-0.6331807508,-2.7050365473

H,0,2.4464725746,-1.5599257412,-2.9537869379

H,0,3.7452542253,2.6579355953,-2.7687815146

H,0,5.33263677,1.7543215702,-5.8043811019

H,0,3.6526987193,1.2885348183,-6.2172830897

H,0,4.3559352452,2.7958185214,-6.8840505323

H,0,5.6271434187,3.7448778595,-4.1772982293

H,0,4.8103455344,4.6261897868,-5.5060135854

H,0,4.1444481376,4.6933123873,-3.8484839849

H,0,2.5261139463,4.5121895872,-6.3979942571

H,0,1.7917921472,2.8409199235,-6.1205722109

H,0,1.7025671126,5.2330418057,-4.1414345896

H,0,0.7751561533,2.2817328888,-3.9603882233

H,0,0.7868068391,3.5224937541,-2.5840305481

Cation/N12/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2N12

parent sm conf 2

N12/6-31G*

E(RN12) = -519.370120061

Zero-point correction= 0.241625 (Hartree/Particle)

Thermal correction to Energy= 0.254409

Thermal correction to Enthalpy= 0.255353

Thermal correction to Gibbs Free Energy= 0.202643

Sum of electronic and ZPE= -519.128495

Sum of electronic and thermal Energies= -519.115711

Sum of electronic and thermal Enthalpies= -519.114767

Sum of electronic and thermal Free Energies= -519.167477

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	159.644	47.072	110.937

C,0,2.0693624114,-0.826735041,-2.2909997007

O,0,2.8064644555,0.3910494327,-2.4372418608

C,0,2.7836144465,0.960275659,-3.6254962199

O,0,2.1978976052,0.5330626786,-4.5935661753

C,0,3.6091030077,2.2311816792,-3.5647845136

N,0,3.7095908004,2.9896712112,-4.8486298422

C,0,4.4036552881,2.1707538984,-5.8886983733

C,0,4.5183011185,4.2158805194,-4.5792579416

C,0,2.3327333353,3.4001914924,-5.3873340375

C,0,1.4956115765,4.1405063755,-4.4074346088

C,0,1.2032425912,5.4344107797,-4.5308925466

H,0,2.2818971901,-1.1759089232,-1.2885874733

H,0,1.0075835416,-0.6317159765,-2.4115605567

H,0,2.3966527867,-1.5518029303,-3.0299190452

H,0,4.6194798172,1.9829015174,-3.2508074657

H,0,3.1905285347,2.8963751551,-2.8148614811

H,0,3.8185085826,1.2799104661,-6.07308101

H,0,4.4863479581,2.7656242327,-6.7910388045

H,0,5.3912550714,1.9137069111,-5.5219890913

H,0,5.477772567,3.9206029587,-4.1703597297

H,0,4.6594028669,4.7458490933,-5.5142578778

H,0,3.9812286754,4.8404324406,-3.8754474012

H,0,2.543492918,3.9998697861,-6.2670982487

H,0,1.8642342176,2.4688445687,-5.6882927384

H,0,1.0578805687,3.568139052,-3.5998993158

H,0,1.5964210801,6.0348103394,-5.340336609

H,0,0.5467689872,5.9294306236,-3.8304503317

TS N12 /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentN12

parent ts exo s-cis

N12/6-31G*

E(RN12) = -518.859025806

Zero-point correction= 0.223923 (Hartree/Particle)

Thermal correction to Energy= 0.236612

Thermal correction to Enthalpy= 0.237556

Thermal correction to Gibbs Free Energy= 0.185827

Sum of electronic and ZPE= -518.635102

Sum of electronic and thermal Energies= -518.622414

Sum of electronic and thermal Enthalpies= -518.621469

Sum of electronic and thermal Free Energies= -518.673198

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.476	46.954	108.873

C,0,2.0490754923,-0.8202855069,-2.378918837

O,0,2.7342699992,0.4095184195,-2.4793800431

C,0,2.8104394534,0.9437152042,-3.7336248204

C,0,3.4795834048,2.1904879947,-3.7123869101

N,0,3.8016935943,2.8913013774,-4.8569241793

C,0,4.6655550566,4.0398059666,-4.5734471815

O,0,2.3226615837,0.3586069398,-4.7040651241

C,0,4.2938783878,2.1146141628,-6.0014822734

C,0,2.1588480051,3.781536903,-5.6633740417

C,0,1.5197493012,4.2672374683,-4.5069511675

C,0,0.9517219228,3.4040540935,-3.6220041577

H,0,2.0892314482,-1.1014986488,-1.331178372

H,0,1.0109620185,-0.7256565957,-2.6954215837

H,0,2.5240920646,-1.5896732011,-2.9863934128

H,0,3.7382992329,2.6408111724,-2.7723104552

H,0,5.3027675852,1.7603653875,-5.7918744266

H,0,3.6329878472,1.2707460757,-6.1541514988

H,0,4.309376853,2.7517521444,-6.8809088502

H,0,5.6211398458,3.6954426987,-4.1799050337

H,0,4.8283095699,4.6019937125,-5.4868517795

H,0,4.1795941225,4.6747575992,-3.8396880426

H,0,2.5868118889,4.4702649037,-6.3792910895

H,0,1.8070636777,2.8485678231,-6.0816725312

H,0,1.6868628046,5.2968150047,-4.2134599841

H,0,0.7112737352,2.3933106164,-3.9149505409

H,0,0.5980051046,3.7288692844,-2.6534236632

Cation/N12SX/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2N12SX

parent sm conf 2

N12SX/6-31G*

E(RN12SX) = -519.225340548

Zero-point correction= 0.245635 (Hartree/Particle)

Thermal correction to Energy= 0.258387

Thermal correction to Enthalpy= 0.259331

Thermal correction to Gibbs Free Energy= 0.206316

Sum of electronic and ZPE= -518.979705

Sum of electronic and thermal Energies= -518.966954

Sum of electronic and thermal Enthalpies= -518.966009

Sum of electronic and thermal Free Energies= -519.019024

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.140	46.381	111.579

C,0,2.0562441811,-0.8101113042,-2.2769408091

O,0,2.7892076254,0.4100953084,-2.4307669779

C,0,2.7834968007,0.9646651572,-3.6261628454

O,0,2.2078879347,0.5260615174,-4.5938503898

C,0,3.6142948463,2.2305015704,-3.5757234577

N,0,3.7094841649,2.9895402465,-4.8589049351

C,0,4.4058618069,2.1749494645,-5.9027436964

C,0,4.5209116361,4.2155375503,-4.5876463182

C,0,2.3387959085,3.4022207212,-5.3976529024

C,0,1.4895077728,4.1181758801,-4.4041243941

C,0,1.2028196126,5.4136776323,-4.4965873271

H,0,2.1849475624,-1.0999904892,-1.2408793037

H,0,1.0058667076,-0.6433998364,-2.5008893963

H,0,2.4581086681,-1.570997414,-2.94087206

H,0,4.6258538726,1.9720088542,-3.2691879871

H,0,3.2056171774,2.8946548067,-2.8178895742

H,0,3.8261683233,1.2797743606,-6.0906431187

H,0,4.4852150663,2.7716251764,-6.8059493879

H,0,5.3971145439,1.9205396477,-5.5400448482

H,0,5.4859042158,3.9174630823,-4.1903475916

H,0,4.6541407465,4.7535363129,-5.5206192089

H,0,3.9923636656,4.8369506672,-3.8728015368

H,0,2.5487228074,4.0267691632,-6.2618736083

H,0,1.8697947514,2.4807636325,-5.7283328605

H,0,1.043921468,3.5247739116,-3.6145140687

H,0,1.6054222514,6.0339116227,-5.2877631358

H,0,0.5413578819,5.8936207574,-3.7886112604

TS N12SX /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentN12SX

parent ts exo s-cis

N12SX/6-31G*

E(RN12SX) = -518.702689131

Zero-point correction= 0.227999 (Hartree/Particle)

Thermal correction to Energy= 0.240447

Thermal correction to Enthalpy= 0.241391

Thermal correction to Gibbs Free Energy= 0.190073

Sum of electronic and ZPE= -518.474690

Sum of electronic and thermal Energies= -518.462242

Sum of electronic and thermal Enthalpies= -518.461298

Sum of electronic and thermal Free Energies= -518.512616

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 150.883 45.859 108.009

C,0,2.0354877349,-0.8004177525,-2.3548270511

O,0,2.7090309373,0.4379353926,-2.476326576

C,0,2.7766300822,0.9589915667,-3.7313466413

C,0,3.3870970636,2.2406442464,-3.7214866376

N,0,3.770800411,2.9073320703,-4.8712943284

C,0,4.6468972515,4.0436032668,-4.5746232581

O,0,2.3058012098,0.3522465495,-4.6945766119

C,0,4.2782297406,2.1150453827,-5.998356289

C,0,2.1527298599,3.8258004201,-5.6885034773

C,0,1.5307091608,4.2554871924,-4.5093572803

C,0,1.0720582713,3.3055370504,-3.6391989501

H,0,2.0766919133,-1.0647083282,-1.301945607

H,0,0.9970190545,-0.7179210948,-2.674383178

H,0,2.5208450307,-1.5733210211,-2.9496218665

H,0,3.7012800612,2.6600013709,-2.7822775499

H,0,5.2778618294,1.7440439005,-5.7669845835

H,0,3.6102091454,1.2802865896,-6.171239081

H,0,4.3252605947,2.7500242149,-6.8803206207

H,0,5.5855776519,3.6897707663,-4.1462369962

H,0,4.8503021892,4.5925707967,-5.4899705923

H,0,4.149785493,4.699156285,-3.8644626444

H,0,2.5908945663,4.5382148577,-6.3768752926

H,0,1.8106312451,2.9041123066,-6.1428261101

H,0,1.7078224175,5.265878805,-4.1577425788

H,0,0.7699903031,2.3329034338,-4.000834061

H,0,0.7746107819,3.5542427317,-2.6284221365

Cation/ SOGGA11/6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2SOGGA11

parent sm conf 2

SOGGA11/6-31G*

E(RSOGGA11) = -519.511656104

Zero-point correction= 0.238437 (Hartree/Particle)

Thermal correction to Energy= 0.251627

Thermal correction to Enthalpy= 0.252571

Thermal correction to Gibbs Free Energy= 0.198804

Sum of electronic and ZPE= -519.273219

Sum of electronic and thermal Energies= -519.260029

Sum of electronic and thermal Enthalpies= -519.259085

Sum of electronic and thermal Free Energies= -519.312852

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 157.898 48.019 113.162

C,0,1.9820036548,-0.7625748243,-2.2069933209

O,0,2.6997561064,0.4624778074,-2.4017430785

C,0,2.8065637154,0.905543301,-3.653163056

O,0,2.3274245157,0.3840177386,-4.6358261264

C,0,3.6674515272,2.1700688296,-3.6121448478

N,0,3.7362689209,2.9869346089,-4.8796345008

C,0,4.4296816875,2.2235036397,-5.9788337023

C,0,4.5567612281,4.2113811565,-4.5697834717

C,0,2.342227481,3.425410937,-5.3960855501

C,0,1.476682946,4.1080205336,-4.3896226502

C,0,1.1320607194,5.3949704568,-4.4691662196

H,0,1.9792150731,-0.9360317997,-1.1295661817

H,0,0.9568555966,-0.6734240805,-2.5795750521

H,0,2.4839072826,-1.5879926048,-2.7217461326

H,0,4.6936309659,1.8852929563,-3.3644480054

H,0,3.311547633,2.8237849162,-2.8167502212

H,0,3.8495256684,1.3345307002,-6.2120558916

H,0,4.5023931214,2.8735534331,-6.8509317524

H,0,5.4279317738,1.951831097,-5.6330730594

H,0,5.5341961279,3.8936586196,-4.2063556919

H,0,4.669271638,4.7892487369,-5.4870333996

H,0,4.0415138055,4.8035006432,-3.8154887125

H,0,2.5559069586,4.0758663944,-6.2446323738

H,0,1.8773626679,2.5091794745,-5.7591571107

H,0,1.0565554752,3.4898110527,-3.5991799926

H,0,1.5077732133,6.045356907,-5.2565309771

H,0,0.4445624962,5.8393973688,-3.7528019215

TS SOGGA11 /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentRSOGGA11

parent ts exo s-cis

SOGGA11/6-31G*

E(RSOGGA11) = -519.003299829

Zero-point correction= 0.221265 (Hartree/Particle)

Thermal correction to Energy= 0.234291

Thermal correction to Enthalpy= 0.235235

Thermal correction to Gibbs Free Energy= 0.182513

Sum of electronic and ZPE= -518.782035

Sum of electronic and thermal Energies= -518.769009

Sum of electronic and thermal Enthalpies= -518.768065

Sum of electronic and thermal Free Energies= -518.820786

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	147.020	47.582	110.962

C,0,2.0564797802,-0.8334529944,-2.32627083

O,0,2.7798781402,0.3718212073,-2.4720904918

C,0,2.8464312617,0.8687242218,-3.7596730876

C,0,3.5079333273,2.1301560287,-3.7458859324

N,0,3.8106087223,2.8758132106,-4.8738969335

C,0,4.6734602068,4.0320772245,-4.5564802909

O,0,2.3662910416,0.2513817392,-4.7157485035

C,0,4.3217330871,2.1466528706,-6.0553619746

C,0,2.1641414241,3.7846330871,-5.6572731194

C,0,1.5092894797,4.281797856,-4.5023037846

C,0,0.8617998268,3.4627421462,-3.6298899216

H,0,2.0818860756,-1.0816607265,-1.2609291967

H,0,1.0134859762,-0.723010491,-2.6509419358

H,0,2.5039766371,-1.6529530331,-2.9024837616

H,0,3.7272461067,2.5898336618,-2.7954762567

H,0,5.336361283,1.7919793432,-5.845972402

H,0,3.6715317448,1.299571084,-6.2539206387

H,0,4.3410592722,2.8240478598,-6.9106085252

H,0,5.6437616676,3.6767147101,-4.1948353037

H,0,4.8149408403,4.6345792767,-5.4544068259

H,0,4.1936405708,4.6348907035,-3.7856811625

H,0,2.6019405668,4.4815175471,-6.3671436283

H,0,1.7874668747,2.866108758,-6.0968123791

H,0,1.6982949106,5.3148221019,-4.2117654923

H,0,0.6137750433,2.4398303315,-3.8917277591

H,0,0.4868401325,3.8288432755,-2.6764598624

Cation/ SOGGA11X /6-31G*/PCM-Conf2

/home/bibaswanbiswas/c8/newMinnFunc/SM2SOGGA11X

parent sm conf 2

SOGGA11X/6-31G*

E(RSOGGA11X) = -519.355548556

Zero-point correction= 0.246551 (Hartree/Particle)

Thermal correction to Energy= 0.259250

Thermal correction to Enthalpy= 0.260194

Thermal correction to Gibbs Free Energy= 0.207270

Sum of electronic and ZPE= -519.108998

Sum of electronic and thermal Energies= -519.096299

Sum of electronic and thermal Enthalpies= -519.095355

Sum of electronic and thermal Free Energies= -519.148278

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	162.682	46.145	111.387

C,0,2.0445472635,-0.8050728211,-2.2729718075

O,0,2.7943086836,0.4170624491,-2.418203596

C,0,2.7801603675,0.9681703745,-3.6191716474

O,0,2.1951968675,0.5325976289,-4.5838313072

C,0,3.6209361403,2.236052061,-3.5738105675

N,0,3.7143797523,2.9911294324,-4.8645330794

C,0,4.4144901202,2.1694072974,-5.9070359922

C,0,4.5304587942,4.2206370186,-4.5965052789

C,0,2.3431000174,3.4035840898,-5.4099054623

C,0,1.4766734171,4.1005745696,-4.4061185134

C,0,1.1912214898,5.4012364499,-4.476681724

H,0,2.1787095322,-1.0982353716,-1.2340845878

H,0,0.9915819716,-0.6229906338,-2.4917567908

H,0,2.4416943276,-1.5665317015,-2.9454387939

H,0,4.6369742361,1.9718831901,-3.2705668252

H,0,3.2145459495,2.9071689653,-2.8141568103

H,0,3.8332861621,1.2688173632,-6.091518739

H,0,4.4926701606,2.7654193963,-6.8164920727

H,0,5.4102421807,1.9181929814,-5.540310264

H,0,5.4994826802,3.9191214035,-4.1987937577

H,0,4.6628401223,4.7574411625,-5.5357420861

H,0,4.0021646628,4.846188684,-3.8779831236

H,0,2.5580830294,4.0484445339,-6.2641102073

H,0,1.8798757388,2.4820020401,-5.7616746725

H,0,1.0167590748,3.4877322577,-3.6331617476

H,0,1.606991312,6.039209732,-5.2531605665

H,0,0.5176579456,5.8680754468,-3.7646029797

TS SOGGA11X /6-31G*/PCM

/home/bibaswanbiswas/c8/newMinnFunc/TSparentRSOGGA11X

parent ts exo s-cis

SOGGA11X/6-31G*

E(RSOGGA11X) = -518.827279415

Zero-point correction= 0.228862 (Hartree/Particle)

Thermal correction to Energy= 0.241196

Thermal correction to Enthalpy= 0.242141

Thermal correction to Gibbs Free Energy= 0.191092

Sum of electronic and ZPE= -518.598417

Sum of electronic and thermal Energies= -518.586083

Sum of electronic and thermal Enthalpies= -518.585139

Sum of electronic and thermal Free Energies= -518.636188

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.353	45.547	107.442

C,0,2.0392457432,-0.8076916123,-2.3491661653

O,0,2.7124331903,0.4409415815,-2.4664164491

C,0,2.7679561999,0.9573465487,-3.7272756887

C,0,3.3682397852,2.2521112242,-3.7190483075

N,0,3.760402671,2.9129515553,-4.8760681687

C,0,4.6508850053,4.042684253,-4.57361537

O,0,2.2959892859,0.3462591075,-4.6877666119

C,0,4.2782730798,2.110791222,-5.9978119679

C,0,2.1435972704,3.8414664962,-5.6996449459

C,0,1.5210129559,4.2647360704,-4.5141626895

C,0,1.085143923,3.2943627455,-3.6447188412

H,0,2.0837639747,-1.0668626306,-1.2906734721

H,0,0.997172443,-0.7261969259,-2.6701062895

H,0,2.533846945,-1.5798093337,-2.9443437534

H,0,3.7004796442,2.6657470546,-2.7781122655

H,0,5.2725229504,1.7221408992,-5.7498473071

H,0,3.597851255,1.2844575228,-6.1887392907

H,0,4.3500081925,2.7531372709,-6.8790720819

H,0,5.5885101513,3.6780969951,-4.1394626632

H,0,4.8630696591,4.59170167,-5.4928960097

H,0,4.1547510374,4.7058230514,-3.8622160849

H,0,2.5836476199,4.5615178555,-6.3865471614

H,0,1.7997449393,2.9189713456,-6.162500555

H,0,1.7071996006,5.2735070392,-4.1486469551

H,0,0.7638379763,2.3283292147,-4.0211907286

H,0,0.7946685018,3.5309407794,-2.623990176

Structures for Reactions of Alanineprenyl Ammonium Salt

TSCleavageA/ UB3LYP-D2/6-31G*/PCM

/home/bibaswanbiswas/c11/cleavageAB3D2SB

trimethyl pure cleavage conf A

UB3LYP/6-31G*

E(UB3LYP) = -636.975962660

Zero-point correction= 0.306380 (Hartree/Particle)

Thermal correction to Energy= 0.323922

Thermal correction to Enthalpy= 0.324867

Thermal correction to Gibbs Free Energy= 0.261199

Sum of electronic and zero-point Energies= -636.669583

Sum of electronic and thermal Energies= -636.652040

Sum of electronic and thermal Enthalpies= -636.651096

Sum of electronic and thermal Free Energies= -636.714763

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	203.264	63.657	133.999

C	0.96186	0.05852	-1.11585
C	2.23451	-0.54129	-1.02972
C	3.39921	0.03075	-0.56925
C	3.51838	1.46587	-0.13722
C	4.67058	-0.76706	-0.49488
N	-0.15945	-0.24764	0.82847
C	0.79745	0.38775	1.74175
C	-1.41773	0.34013	0.71215
C	-1.64495	1.68974	1.34161
C	-2.33513	-0.2014	-0.24274

C	-0.07123	-1.71616	0.94601
H	4.52065	-1.80463	-0.81505
H	5.45483	-0.31884	-1.1254
H	5.07099	-0.77378	0.53108
H	4.27061	1.98828	-0.74808
H	2.57645	2.01639	-0.2078
H	3.87	1.52592	0.90379
H	2.29362	-1.59289	-1.3139
H	0.83883	1.12812	-0.98334
H	0.14725	-0.46113	-1.60582
H	0.84583	1.46082	1.55765
H	0.50921	0.20546	2.78626
H	1.78074	-0.04876	1.55089
H	0.96555	-2.00953	0.76267
H	-0.36575	-2.01269	1.9625
H	-0.72796	-2.17443	0.21135
H	-2.69582	1.96685	1.25076
H	-1.37769	1.69542	2.40647
H	-1.04977	2.48384	0.85964
O	-2.14357	-1.15262	-1.02073
O	-3.54574	0.4606	-0.24836
C	-4.49635	-0.02563	-1.19845

H -5.37992 0.60622 -1.08043

H -4.10769 0.05236 -2.22009

H -4.75037 -1.07316 -1.00045

TSCleavageB/ UB3LYP-D2/6-31G*/ PCM

/home/bibaswanbiswas/c11/cleavageBB3D2SB

trimethyl pure cleavage conf B

UB3LYP/6-31G*

E(UB3LYP) = -636.976342409

Zero-point correction= 0.306776 (Hartree/Particle)

Thermal correction to Energy= 0.324136

Thermal correction to Enthalpy= 0.325081

Thermal correction to Gibbs Free Energy= 0.262236

Sum of electronic and ZPE= -636.669566

Sum of electronic and thermal Energies= -636.652206

Sum of electronic and thermal Enthalpies= -636.651262

Sum of electronic and thermal Free Energies= -636.714106

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.399	63.496	132.268

C,0,0.872752882,-0.1728587055,-0.9621135773

C,0,2.2132613596,-0.6034704406,-0.8936508531

C,0,3.2954914666,0.1615617617,-0.5204870944

C,0,3.1953871901,1.6169224157,-0.1541050529

C,0,4.6764237146,-0.4274655639,-0.4692327916

N,0,-0.1531187028,-0.3376171624,1.0517264683

C,0,0.885524265,0.1799987806,1.9611467536

C,0,-1.3653416886,0.3462921175,0.9509834669

C,0,-2.6200090805,-0.4478824324,0.6960161764

C,0,-1.3278519825,1.7618122989,0.7632261062

C,0,-0.219054196,-1.8020164959,1.1583648557

H,0,4.6811108953,-1.4859345184,-0.7541818128

H,0,5.3606376409,0.1155024686,-1.1404861591

H,0,5.1049325726,-0.3359392166,0.5412906538

H,0,3.6811499388,2.242565822,-0.9198575582

H,0,2.1640375766,1.9574621605,-0.0276407449

H,0,3.73631287,1.8058485073,0.7851569425

H,0,2.408888652,-1.6535462354,-1.1155033037

H,0,0.6203996585,0.8789900306,-0.9188992882

H,0,0.1233612353,-0.8350748306,-1.3824390426

H,0,0.9098348206,1.2641029922,1.9048136664

H,0,0.6564907127,-0.1491278083,2.9843484124

H,0,1.8491039273,-0.2310980077,1.6505648484

H,0,0.7969758786,-2.1907191648,1.0586038325

H,0,-0.6299364426,-2.0957134823,2.1341728129

H,0,-0.8388507763,-2.2155876131,0.3625780878

H,0,-3.4852284107,0.2157789245,0.7116017041

H,0,-2.6045627682,-0.9494849493,-0.2865844199

H,0,-2.77456105,-1.2309943697,1.4497252153

O,0,-0.3189578801,2.4851691844,0.6599410403

O,0,-2.5866848245,2.3233117166,0.6923076181

C,0,-2.6078423368,3.7349978289,0.4713573216

H,0,-3.6642704646,4.0123238703,0.4405246306

H,0,-2.099059324,4.2685511301,1.2821139524

H,0,-2.1203973287,3.9926879865,-0.4758198676

TSCleavageA/ UM062X/6-31G*/PCM

/home/bibaswanbiswas/c11/cleavageAM062XSB

trimethyl pure cleavage conf A

UM062X/6-31G*

E(UM062X) = -636.614382233

Zero-point correction= 0.309673 (Hartree/Particle)

Thermal correction to Energy= 0.327207

Thermal correction to Enthalpy= 0.328151

Thermal correction to Gibbs Free Energy= 0.264503

Sum of electronic and ZPE= -636.304709

Sum of electronic and thermal Energies= -636.287176

Sum of electronic and thermal Enthalpies= -636.286232

Sum of electronic and thermal Free Energies= -636.349879

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	205.325	63.518	133.958

C,0,0.9507872778,0.0350160376,-1.0699864052

C,0,2.2372713318,-0.5447608178,-1.0078149658

C,0,3.4000723239,0.0450081421,-0.582448903

C,0,3.5086078426,1.4828491599,-0.1645613874

C,0,4.6818456566,-0.7338274147,-0.52575822

N,0,-0.1685744879,-0.269482346,0.8491206837

C,0,0.779346658,0.3503788638,1.7754044303

C,0,-1.4074764822,0.3353680996,0.7191925326

C,0,-1.6282153773,1.6928077109,1.3232652317

C,0,-2.330644737,-0.2052535351,-0.2311742876

C,0,-0.1008117135,-1.7349295241,0.9557577721

H,0,4.5414088782,-1.7720212755,-0.8380848072

H,0,5.446608044,-0.2802793067,-1.1701948155

H,0,5.0965980532,-0.7327920482,0.4911366314

H,0,4.279598364,1.9936766555,-0.7557221038

H,0,2.5745419416,2.0370668036,-0.2754084118

H,0,3.8233752955,1.5568680822,0.8850243676

H,0,2.3036375106,-1.5960675264,-1.2909369962

H,0,0.8117828012,1.105886779,-0.9581578047

H,0,0.1470194547,-0.4951675505,-1.5681000675

H,0,0.8474902442,1.4224059852,1.5934978576

H,0,0.4729811992,0.1734187572,2.813902463

H,0,1.7595686441,-0.1007057278,1.6058757236

H,0,0.9355164429,-2.0400976309,0.7966459891

H,0,-0.4200171826,-2.0348470125,1.9613111677

H,0,-0.7442313522,-2.1853350074,0.2064760298

H,0,-2.6756260941,1.9701961694,1.2175392037

H,0,-1.3771277378,1.715911625,2.3891736314

H,0,-1.0299588159,2.4753892174,0.8327171179

O,0,-2.1522139399,-1.1649994016,-0.9894014664

O,0,-3.5177248817,0.4747470681,-0.256209482

C,0,-4.4603748888,-0.000966734,-1.2063715106

H,0,-5.3284286121,0.6519498703,-1.1171153938

H,0,-4.0543865503,0.0486079254,-2.2198565687

H,0,-4.7448141106,-1.034635093,-0.9932512357

TS23/ N12/6-31G*/ exo s-cis /PCM(DMF)

/home/bibaswanbiswas/c11/obscure/me3TSN12normal

trimethyl ts exo s-cis

N12/6-31G*

E(RN12) = -636.780168187

Zero-point correction= 0.308671 (Hartree/Particle)

Thermal correction to Energy= 0.325512

Thermal correction to Enthalpy= 0.326456

Thermal correction to Gibbs Free Energy= 0.265870

Sum of electronic and ZPE= -636.471498

Sum of electronic and thermal Energies= -636.454656

Sum of electronic and thermal Enthalpies= -636.453712

Sum of electronic and thermal Free Energies= -636.514298

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	204.262	62.915	127.514

C,0,-0.1715715268,0.7048441087,0.52463348

C,0,0.3956347491,0.4590627633,1.7919959173

C,0,1.7360901208,0.4423714881,2.0614517443

C,0,2.7769006932,0.4468338518,0.9906072038

C,0,2.2259502437,0.3323638344,3.4679095638

N,0,-0.4345184883,2.7541455998,0.4109040105

C,0,-1.866494884,2.8470203983,0.7195816899

C,0,0.384799222,3.4776027871,1.2841602816

C,0,-0.1478383238,3.8051260704,2.6428463348

C,0,1.7392138823,3.7227458393,0.9563546077

C,0,-0.2414480376,2.9799460698,-1.0296467312

H,0,1.4149352407,0.3554253238,4.1927057986

H,0,2.7911192029,-0.5920334297,3.6158440676

H,0,2.9173654446,1.1445741005,3.7045900093

H,0,2.5064872338,-0.213981913,0.166205217

H,0,2.9009695793,1.4471133222,0.5580837988

H,0,3.740562466,0.1222096793,1.3792003032

H,0,-0.2838329321,0.3860838374,2.6339930877

H,0,0.4608833068,0.6202726746,-0.3474395771

H,0,-1.203078142,0.4302262819,0.3558564852

H,0,-2.0703474087,2.4681402897,1.7134149672

H,0,-2.1965267738,3.8832110624,0.6514936257

H,0,-2.4170592711,2.2541617298,-0.0028086891

H,0,-0.815309818,2.2390344361,-1.5780903365

H,0,-0.6016078057,3.9767579663,-1.2859210178

H,0,0.8127462336,2.9045403882,-1.2557974073

H,0,0.6346474704,4.2771392801,3.224664212

H,0,-1.0007413287,4.4879329754,2.6243133688

H,0,-0.468879854,2.913856106,3.1892526878

O,0,2.377506623,3.3526885492,-0.0439797526

O,0,2.3777371766,4.4888818402,1.9042693502

C,0,3.7194135881,4.8127539821,1.6246494253

H,0,4.0439719445,5.4631584531,2.4318383175

H,0,4.3528579387,3.9266841697,1.5946605451

H,0,3.8158612348,5.3322670838,0.6717774105

TSCleavageA/ UM06/6-31G*/PCM

/home/bibaswanbiswas/c11/cleavageAM06SB

trimethyl pure cleavage conf A

UM06/6-31G*

E(UM06) = -636.475361474

Zero-point correction= 0.305133 (Hartree/Particle)

Thermal correction to Energy= 0.322776

Thermal correction to Enthalpy= 0.323720

Thermal correction to Gibbs Free Energy= 0.259429

Sum of electronic and ZPE= -636.170229

Sum of electronic and thermal Energies= -636.152585

Sum of electronic and thermal Enthalpies= -636.151641

Sum of electronic and thermal Free Energies= -636.215932

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	202.545	64.024	135.312

C,0,0.9542306862,0.0057639336,-1.0119187567

C,0,2.24991062,-0.5521893838,-0.9587657612

C,0,3.4143391943,0.0691959403,-0.588011801

C,0,3.5196206388,1.5193088512,-0.2441285314

C,0,4.7006349861,-0.6876519124,-0.5297595624

N,0,-0.1680881961,-0.2984112868,0.8474078459

C,0,0.7582583438,0.2847245778,1.8139019715

C,0,-1.4127142358,0.324818327,0.7217473897

C,0,-1.6043156566,1.6846435698,1.3143904115

C,0,-2.326531863,-0.1960708768,-0.2428130057

C,0,-0.1469649522,-1.7636127417,0.9630595076

H,0,4.5747297917,-1.743610966,-0.7967426981

H,0,5.45139678,-0.2498371442,-1.2064663584

H,0,5.1422426107,-0.640521849,0.4784295576

H,0,4.2887187345,2.0061931665,-0.8632268107

H,0,2.5833812274,2.0720088469,-0.3760087642

H,0,3.8437528158,1.6515787335,0.800265847

H,0,2.3264121228,-1.6156101964,-1.2065932235

H,0,0.8083222247,1.0826874072,-0.9225212361

H,0,0.1597005882,-0.5265768672,-1.5307055912

H,0,0.8417677235,1.3641770575,1.6689998824

H,0,0.4231490225,0.0823902582,2.8424318002

H,0,1.7445683201,-0.1680724317,1.6635773181

H,0,0.8818046581,-2.1133481363,0.8251595295

H,0,-0.496086824,-2.0520801198,1.9654744365

H,0,-0.7946622288,-2.1971891793,0.2022061601

H,0,-2.634176194,2.0109755206,1.1553536478

H,0,-1.4111906251,1.7111061375,2.3964554578

H,0,-0.9512192012,2.4494540731,0.8571963065

O,0,-2.1502692076,-1.1454088397,-1.0153814736

O,0,-3.5149625173,0.4878859035,-0.2601251289

C,0,-4.4579344396,0.0277272255,-1.2099813934

H,0,-5.3302782647,0.6785531581,-1.1104547509

H,0,-4.0625064515,0.0905759203,-2.230935972

H,0,-4.7476092315,-1.012191677,-1.0160302503

TS23/ UM062X/6-31G*/ endo s-cis /PCM

/home/bibaswanbiswas/c11/allme3NCM062XSB

endo s-cis isomer of trimethylalanine system

um062X/6-31G*

E(UM062X) = -636.627660384

Zero-point correction= 0.311847 (Hartree/Particle)

Thermal correction to Energy= 0.328356

Thermal correction to Enthalpy= 0.329300

Thermal correction to Gibbs Free Energy= 0.269695

Sum of electronic and ZPE= -636.315814

Sum of electronic and thermal Energies= -636.299305

Sum of electronic and thermal Enthalpies= -636.298361

Sum of electronic and thermal Free Energies= -636.357965

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	206.046	62.322	125.449

C,0,-0.1804468171,0.4762427891,0.2513172089

C,0,0.0990370625,0.1782666755,1.5850693798

C,0,1.3390772718,0.3893285586,2.1528033852

C,0,1.501886509,0.3106574506,3.6459649546

C,0,0.8669272977,2.9180892638,1.3790320534

C,0,2.2252721579,3.3728523419,0.9169020567

C,0,2.6300593947,0.2975170779,1.3884084469

N,0,-0.0832557506,2.5796879381,0.4199190688

C,0,0.2341333775,2.9758628389,-0.9612075318

C,0,0.4968056772,3.0155573952,2.7644622146

O,0,1.5308611425,3.4877948811,3.5368280676

C,0,1.2227782525,3.6426642416,4.9148259471

C,0,-1.5052520339,2.8668294854,0.7023011221

O,0,-0.5803597538,2.7468082195,3.298964544

H,0,0.5520682817,0.4889300261,4.1579692105

H,0,1.8849990478,-0.6743203774,3.946338628

H,0,2.2273000721,1.0564665427,3.9921900791

H,0,3.3544030512,1.0376665688,1.7446332732

H,0,3.07987674,-0.6910173437,1.5571550963

H,0,2.5116803712,0.4278035166,0.310797452

H,0,-0.7470266118,0.0887281193,2.2650807637

H,0,0.5996965009,0.4279387452,-0.5033866773

H,0,-1.188841474,0.3451760265,-0.1328484942

H,0,-1.8265639984,2.3174464595,1.5798620599

H,0,-1.636658058,3.9403364949,0.8778912431

H,0,-2.0868073896,2.5673921752,-0.1709398117

H,0,-0.4973600247,2.5141216083,-1.6259318657

H,0,0.1831840817,4.0656783949,-1.0680439821

H,0,1.2265886281,2.6309378731,-1.2447061105

H,0,2.1851771522,4.336185587,0.390446258

H,0,2.8822905893,3.4911054292,1.7764945105

H,0,2.7043442685,2.657654973,0.2393177076

H,0,2.136843684,4.0080183151,5.3836228552

H,0,0.4143453607,4.3650919276,5.0560919618

H,0,0.9256649393,2.6914347808,5.3631239248

TS23/ UM06/6-31G*/ endo s-trans /PCM

/home/bibaswanbiswas/c11/allme3NTM06SB

endo s-trans isomer of trimethylalanine system

um06/6-31G*

E(UM06) = -636.483393128

Zero-point correction= 0.308783 (Hartree/Particle)

Thermal correction to Energy= 0.324717

Thermal correction to Enthalpy= 0.325661

Thermal correction to Gibbs Free Energy= 0.268103

Sum of electronic and ZPE= -636.174611

Sum of electronic and thermal Energies= -636.158676

Sum of electronic and thermal Enthalpies= -636.157732

Sum of electronic and thermal Free Energies= -636.215290

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.763	62.069	121.142

C,0,-0.0473749285,0.4816483307,0.0764154437

C,0,0.1192851936,0.085816142,1.4065039041

C,0,1.2920684298,0.1838640465,2.1158664475

C,0,2.6490573679,0.2605484762,1.4991386548

C,0,1.3066643629,0.0277928524,3.5985877754

N,0,-0.1333667834,2.6043766603,0.3704621091

C,0,-1.5776854671,2.7684042343,0.6152726887

C,0,0.7787260635,2.9893720367,1.3536863828

C,0,0.5439873816,2.9863597736,2.7666292153

O,0,1.3915707633,3.3008818531,3.611307226

C,0,2.1510157495,3.3982863344,0.9167004882

C,0,0.1745950013,3.0784508521,-0.9869558254

O,0,-0.718792924,2.6510637042,3.1803619756

C,0,-0.9694409404,2.82330213,4.5629967697

H,0,0.3198420176,-0.2300468464,4.0024817747

H,0,2.0266520812,-0.7413409146,3.9175805472

H,0,1.6320717551,0.9763869404,4.0635657645

H,0,3.2447781445,1.0648318605,1.9572770211

H,0,3.197549849,-0.6748285654,1.6937988526

H,0,2.6393460971,0.4174672556,0.415427533

H,0,-0.7902513682,-0.0879550123,1.9885501357

H,0,0.8072386322,0.5345146281,-0.5978277407

H,0,-1.0057472905,0.3285137455,-0.4190512666

H,0,-1.9025882839,2.1331340773,1.4354739147

H,0,-1.7982542369,3.8160870962,0.8616273066

H,0,-2.1131588162,2.4910404663,-0.2976016384

H,0,-0.5029723563,2.5868737462,-1.6912948764

H,0,0.0334417746,4.1672627712,-1.0525376762

H,0,1.2001082291,2.8329887768,-1.2676650508

H,0,2.1548529548,4.3241484627,0.3211205706

H,0,2.7584946091,3.5752848259,1.8074562216

H,0,2.665458134,2.6324253361,0.3144106194

H,0,-2.0164738276,2.5473411979,4.7150066531

H,0,-0.3272019684,2.1832416425,5.1784128639

H,0,-0.8145234003,3.8652320828,4.8688902152

TSCleavageA/ UM06/6-31+G/ PCM**

/home/bibaswanbiswas/c11/cleavageAM06PS

trimethyl pure cleavage conf A

UM06/6-31+G**

E(UM06) = -636.521859139

Zero-point correction= 0.303596 (Hartree/Particle)

Thermal correction to Energy= 0.320985

Thermal correction to Enthalpy= 0.321929

Thermal correction to Gibbs Free Energy= 0.258927

Sum of electronic and ZPE= -636.218263

Sum of electronic and thermal Energies= -636.200874

Sum of electronic and thermal Enthalpies= -636.199930

Sum of electronic and thermal Free Energies= -636.262932

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	201.421	64.267	132.600

C,0,0.9923676419,0.0280016999,-1.0227931804

C,0,2.2841265363,-0.5389304493,-0.9591626444

C,0,3.4473439242,0.0799201121,-0.5744867839

C,0,3.5479906647,1.5272665269,-0.2199926923

C,0,4.7326148457,-0.6777528454,-0.5099830016

N,0,-0.1774651443,-0.3058482098,0.8226917602

C,0,0.729735531,0.256321184,1.8239399222

C,0,-1.4151821326,0.3282231636,0.686921027

C,0,-1.5709053579,1.7132273029,1.2329965439

C,0,-2.3606925641,-0.2072754344,-0.2381748119

C,0,-0.1545108663,-1.7741046139,0.9203638649

H,0,4.6063353819,-1.7324469936,-0.7757401282

H,0,5.4833337068,-0.2393781672,-1.1838394175

H,0,5.1668859818,-0.6262943671,0.4995669905

H,0,4.3128633982,2.0179362779,-0.8384919917

H,0,2.6104340248,2.0768138713,-0.3439244844

H,0,3.8768764432,1.6481667757,0.8228225822

H,0,2.3599680536,-1.5993855266,-1.2149888686

H,0,0.8508806323,1.1021873755,-0.9154106182

H,0,0.2055261957,-0.4955017763,-1.5587518535

H,0,0.8457464095,1.3330087177,1.6944017084

H,0,0.3520922401,0.0523435673,2.8361643997

H,0,1.7088307994,-0.2177717248,1.70885191

H,0,0.8812708342,-2.1131318015,0.8255925579

H,0,-0.5432908671,-2.0742167555,1.9038674517

H,0,-0.7637064528,-2.2117493341,0.1318929315

H,0,-2.5828847141,2.0725256015,1.0443934937

H,0,-1.3952963937,1.7697686117,2.3152006224

H,0,-0.8808247267,2.4318737179,0.7591059524

O,0,-2.2182511089,-1.1826852124,-0.9901923876

O,0,-3.5428067701,0.4901778625,-0.2452409183

C,0,-4.5336397268,0.0109941136,-1.1416875489

H,0,-5.3956569516,0.6684377851,-1.0154100199

H,0,-4.1853121001,0.050922041,-2.1791166868

H,0,-4.8173663679,-1.0202580961,-0.9058996804

TS23/ UM062X/6-31G*/ endo s-trans / Gas

/home/bibaswanbiswas/c11/allme3NTM062XSB

endo s-trans isomer of trimethylalanine system

um062X/6-31G*

E(UM062X) = -636.617219503

Zero-point correction= 0.313451 (Hartree/Particle)

Thermal correction to Energy= 0.329430

Thermal correction to Enthalpy= 0.330374

Thermal correction to Gibbs Free Energy= 0.272567

Sum of electronic and ZPE= -636.303769

Sum of electronic and thermal Energies= -636.287789

Sum of electronic and thermal Enthalpies= -636.286845

Sum of electronic and thermal Free Energies= -636.344652

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	206.720	61.600	121.665

C,0,0.0062835006,0.5084784462,0.0103230279

C,0,0.1140253217,0.0868351913,1.3415343534

C,0,1.2403593838,0.2611286523,2.1104218977

C,0,2.6390346254,0.3361341275,1.5701283842

C,0,1.1735761233,0.0986157702,3.600060813

N,0,-0.1230321983,2.5630800213,0.3600411144

C,0,-1.5629934645,2.674950966,0.6669682797

C,0,0.8051226048,2.9302629844,1.3270302519

C,0,0.5847591858,2.9580801219,2.7494984401

O,0,1.4325619367,3.3058893285,3.5670955932

C,0,2.1640369528,3.3822079737,0.8729387045

C,0,0.1325968174,3.101610945,-0.9852842331

O,0,-0.6617727269,2.5862773068,3.1869659773

C,0,-0.8775499708,2.783057501,4.5772472715

H,0,0.1458770578,-0.0435695536,3.9457264222

H,0,1.7782826936,-0.7562888994,3.9301848669

H,0,1.5869115753,0.9940072475,4.087449942

H,0,3.1943769844,1.1535736877,2.0447171423

H,0,3.1700370795,-0.5941474022,1.8137807119

H,0,2.6843001547,0.4678159684,0.4874494467

H,0,-0.8129455637,-0.1318263641,1.8707921428

H,0,0.8959712767,0.589488948,-0.6090806018

H,0,-0.9104084543,0.3141999396,-0.5421394373

H,0,-1.8267976405,1.9906761757,1.4656731667

H,0,-1.7981117092,3.6981201047,0.9768443965

H,0,-2.1178127748,2.4235355366,-0.2389490833

H,0,-0.5536548988,2.6214965498,-1.6851630393

H,0,-0.0311784943,4.1858445028,-0.997840684

H,0,1.1535573492,2.8884100248,-1.2949417734

H,0,2.1338711916,4.3332109223,0.3245290486

H,0,2.7812680609,3.5319695894,1.7581418749

H,0,2.6678474035,2.6508506228,0.2266171261

H,0,-1.912363262,2.4889336747,4.7585254598

H,0,-0.2001187634,2.1692570042,5.1748081529

H,0,-0.7269453581,3.8306033839,4.8499798431

TS23/ UM062X/6-31G*/ exo s-trans / PCM

/home/bibaswanbiswas/c11/allme3XTM062XSB

exo s-trans isomer of trimethylalanine system

um062X/6-31G*

E(UM062X) = -636.624650896

Zero-point correction= 0.313316 (Hartree/Particle)

Thermal correction to Energy= 0.329255

Thermal correction to Enthalpy= 0.330200

Thermal correction to Gibbs Free Energy= 0.272424

Sum of electronic and ZPE= -636.311335

Sum of electronic and thermal Energies= -636.295396

Sum of electronic and thermal Enthalpies= -636.294451

Sum of electronic and thermal Free Energies= -636.352227

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	206.611	61.497	121.600

C,0,-0.275612224,0.7099609689,0.214439431

C,0,0.302817612,0.3601804197,1.44552669

C,0,1.5831002556,0.7226815506,1.7867793782

C,0,2.039390644,0.6992475665,3.2153831741

C,0,2.7041362241,0.8943190753,0.7985286108

N,0,-0.4554111078,2.7460830653,0.4949062461

C,0,-0.2765610898,3.2428718281,-0.8865855921

C,0,-1.8860902857,2.8434829438,0.8551345218

C,0,0.4101048297,3.1667852146,1.5117771601

C,0,1.7458098793,3.6462625811,1.3364796638

O,0,2.1977892277,3.7305886165,0.0473890131

C,0,3.5083518879,4.2583348358,-0.102864373

C,0,-0.1094918889,3.176561683,2.9241078576

O,0,2.496783868,3.9821903707,2.2595481848

H,0,1.2192590409,0.4890392179,3.9074605744

H,0,2.8314295778,-0.0451663056,3.3708237141

H,0,2.4676198657,1.6815971832,3.4620634695

H,0,3.3849438311,1.6852557962,1.1320661847

H,0,3.2891304548,-0.0348798036,0.7603389377

H,0,2.3728044231,1.1338982889,-0.2128177209

H,0,-0.3747260839,0.0907114277,2.2558061041

H,0,0.3467971058,0.7921652527,-0.6718716312

H,0,-1.3055470483,0.4280049291,0.0102956942

H,0,-2.0900850775,2.2556944515,1.7481537836

H,0,-2.1602960558,3.8893718174,1.0286287099

H,0,-2.4790070735,2.4460123738,0.0314345249

H,0,-1.0539942144,2.7887131185,-1.5029499498

H,0,-0.378379038,4.3324232001,-0.9081982907

H,0,0.6989337046,2.9644920792,-1.267471074

H,0,0.7225854268,3.3990292018,3.5912094811

H,0,-0.8857947854,3.9352293966,3.0905355504

H,0,-0.5322718131,2.209618167,3.2230737749

H,0,3.696598895,4.2815676563,-1.1763868304

H,0,3.5725256594,5.2665509791,0.3134781245

H,0,4.2502963729,3.6268538522,0.3923629027

TS23/ UM06/6-31G*/ endo s-cis / PCM

/home/bibaswanbiswas/c11/allme3NCM06SB

endo s-cis isomer of trimethylalanine system

um06/6-31G*

E(UM06) = -636.484358520

Zero-point correction= 0.308491 (Hartree/Particle)

Thermal correction to Energy= 0.324683

Thermal correction to Enthalpy= 0.325627

Thermal correction to Gibbs Free Energy= 0.266985

Sum of electronic and ZPE= -636.175868

Sum of electronic and thermal Energies= -636.159676

Sum of electronic and thermal Enthalpies= -636.158731

Sum of electronic and thermal Free Energies= -636.217373

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.742	62.327	123.422

C,0,-0.1640312234,0.4768482549,0.2603814875

C,0,0.1168982902,0.1722108962,1.5929735355

C,0,1.3560176428,0.2805656923,2.1780481914

C,0,1.5091665717,0.1794089891,3.6599848824

C,0,0.8301649431,3.0253543136,1.3714146958

C,0,2.1994238511,3.4153376121,0.905450222

C,0,2.6456359895,0.2570223272,1.4260975358

N,0,-0.1059411095,2.6375254061,0.4141239939

C,0,0.2124050958,2.9918005678,-0.9731719603

C,0,0.4820757194,3.0587014667,2.7618464358

O,0,1.5471662377,3.4639639549,3.5398119842

C,0,1.248779168,3.6536829011,4.910103271

C,0,-1.5292751903,2.9232173952,0.6666644151

O,0,-0.5972866622,2.8119131377,3.3049379152

H,0,0.5416353373,0.1663220752,4.1752461211

H,0,2.0702253356,-0.7246472321,3.9456110708

H,0,2.0864349612,1.0375773346,4.0395850812

H,0,3.3347483591,1.0327578,1.7922964267

H,0,3.1548594384,-0.7060716664,1.5927982735

H,0,2.5331548463,0.386765047,0.3441484291

H,0,-0.7368025128,0.0778479822,2.2688555559

H,0,0.6173428433,0.4402973545,-0.4981258888

H,0,-1.1751339975,0.3492410881,-0.1241651374

H,0,-1.830690437,2.5021406513,1.622863524

H,0,-1.6834741412,4.012422651,0.6913168342

H,0,-2.1194444883,2.4957945392,-0.1497811959

H,0,-0.5190615185,2.5115568484,-1.6303366634

H,0,0.1591286353,4.0814715912,-1.1153842532

H,0,1.2077330096,2.6420088745,-1.2542033983

H,0,2.1931738294,4.3229072788,0.2815280957

H,0,2.8401087078,3.6144449003,1.7660898308

H,0,2.6969066203,2.6312725823,0.3133193206

H,0,2.1793643197,3.9869347408,5.377367213

H,0,0.4724532937,4.4165143907,5.0471132342

H,0,0.9088672344,2.7258232534,5.3859399211

TS23/ UM062X/6-31G* exo s-cis /PCM

/home/bibaswanbiswas/c11/allme3XCM062XSB

exo s-cis isomer of trimethylalanine system

um062X/6-31G*

E(UM062X) = -636.626820538

Zero-point correction= 0.312284 (Hartree/Particle)

Thermal correction to Energy= 0.328784

Thermal correction to Enthalpy= 0.329728

Thermal correction to Gibbs Free Energy= 0.270034

Sum of electronic and ZPE= -636.314537

Sum of electronic and thermal Energies= -636.298037

Sum of electronic and thermal Enthalpies= -636.297092

Sum of electronic and thermal Free Energies= -636.356787

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	206.315	62.172	125.637

C,0,-0.3466438234,0.6263672319,0.4011987831

C,0,0.2702460329,0.394603681,1.6402136746

C,0,1.5764714181,0.7446195511,1.8883971097

C,0,2.6484855275,0.7597666592,0.8335574088

C,0,2.0967111922,0.8147969383,3.2959669683

N,0,-0.4004384262,2.6956318046,0.4310453921

C,0,-1.8205305623,2.932519804,0.757353468

C,0,0.5021107905,3.1753715635,1.3852994592

C,0,-0.0002425345,3.3515668546,2.793179493

C,0,1.8211162245,3.5890057559,1.0246668788

C,0,-0.1721735806,3.0097838421,-0.9944354387

H,0,1.2957364499,0.7151464293,4.0339770856

H,0,2.8431028965,0.0310869014,3.4824966848

H,0,2.5976175707,1.7795545082,3.4509488406

H,0,3.4010917285,1.5249200373,1.0484571028

H,0,3.1631760803,-0.2109478373,0.8362464023

H,0,2.2724959255,0.9491608913,-0.1727887886

H,0,-0.3802137062,0.2401476698,2.5009713014

H,0,0.2353261695,0.5701974352,-0.5138001395

H,0,-1.3981953612,0.3805248085,0.2756900061

H,0,-2.0735222199,2.476725442,1.7129318998

H,0,-2.0226282476,4.0085432088,0.7955759257

H,0,-2.4338188381,2.4773176396,-0.0208092274

H,0,-0.9345692559,2.4864245001,-1.5743221669

H,0,-0.2633468355,4.0891044929,-1.1554690388

H,0,0.818988065,2.6892787249,-1.2939819264

H,0,0.8371094009,3.5571004234,3.4574990002

H,0,-0.7171142838,4.1781071243,2.8915632536

H,0,-0.4977650305,2.4469220837,3.1625247708

O,0,2.3609636267,3.6017277435,-0.084649857

O,0,2.5409298619,4.0136149048,2.1194678

C,0,3.8451264017,4.4933811604,1.8278860078

H,0,4.2607015706,4.820009209,2.7813506215

H,0,4.4725977609,3.7085763928,1.3970066349

H,0,3.8074970116,5.3325034202,1.1283586092

TSCleavageA/ UB3LYP-D2/6-31+G/ PCM**

/home/bibaswanbiswas/c11/cleavageAB3D2PS

trimethyl pure cleavage conf A

UB3LYP/6-31+G**

E(UB3LYP) = -637.029163479

Zero-point correction= 0.304002 (Hartree/Particle)

Thermal correction to Energy= 0.321694

Thermal correction to Enthalpy= 0.322638

Thermal correction to Gibbs Free Energy= 0.258567

Sum of electronic and zero-point Energies= -636.725161

Sum of electronic and thermal Energies= -636.707469

Sum of electronic and thermal Enthalpies= -636.706525

Sum of electronic and thermal Free Energies= -636.770597

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	201.866	64.199	134.851

C	0.97015	0.07593	-1.12899
C	2.24082	-0.53003	-1.04338
C	3.40525	0.03581	-0.56898
C	3.52406	1.46586	-0.12123
C	4.67356	-0.76628	-0.4895
N	-0.16151	-0.25434	0.82581
C	0.79556	0.3839	1.73999
C	-1.41902	0.33448	0.70547
C	-1.63442	1.69629	1.31545
C	-2.34672	-0.2143	-0.23368

C	-0.06274	-1.72343	0.9424
H	4.5257	-1.79751	-0.82755
H	5.46516	-0.30722	-1.10094
H	5.0563	-0.78766	0.54222
H	4.29355	1.98445	-0.7117
H	2.58907	2.02398	-0.20755
H	3.85417	1.51145	0.92684
H	2.29874	-1.57818	-1.33803
H	0.84653	1.14172	-0.97254
H	0.15672	-0.43863	-1.62628
H	0.84639	1.4558	1.5562
H	0.50464	0.20094	2.78315
H	1.7781	-0.05398	1.55278
H	0.97771	-2.00747	0.76881
H	-0.36075	-2.01955	1.95765
H	-0.70753	-2.19402	0.20561
H	-2.68153	1.98349	1.22234
H	-1.36519	1.71417	2.37841
H	-1.03109	2.47261	0.81732
O	-2.16378	-1.18047	-1.00165
O	-3.55487	0.45576	-0.24677
C	-4.52503	-0.02849	-1.18495

H	-5.39529	0.61969	-1.06445
H	-4.14259	0.03449	-2.20908
H	-4.79272	-1.06787	-0.96771

TS23/ UM06/6-31G*/ exo s-cis /PCM

/home/bibaswanbiswas/c11/allme3XCM06SB

exo s-cis isomer of trimethylalanine system

um06/6-31G*

E(UM06) = -636.484224568

Zero-point correction= 0.308363 (Hartree/Particle)

Thermal correction to Energy= 0.324628

Thermal correction to Enthalpy= 0.325572

Thermal correction to Gibbs Free Energy= 0.266850

Sum of electronic and ZPE= -636.175862

Sum of electronic and thermal Energies= -636.159596

Sum of electronic and thermal Enthalpies= -636.158652

Sum of electronic and thermal Free Energies= -636.217374

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.707	62.325	123.591

C,0,-0.3596457928,0.6022817651,0.5648361268

C,0,0.3659359376,0.4437868886,1.7559747168

C,0,1.7114489264,0.6772257898,1.8788822937

C,0,2.6652157752,0.6553570904,0.7321288603

C,0,2.3420387391,0.8152271056,3.2257442818

N,0,-0.4379026409,2.7088519458,0.4250820902

C,0,-1.873862657,2.9425072091,0.6510900934

C,0,0.4058302294,3.3031054826,1.3710007595

C,0,-0.1418906199,3.4661531525,2.7560375792

C,0,1.7485777001,3.658925252,1.0639045029

C,0,-0.1425070394,2.9030545049,-1.0049715224

H,0,1.6044670618,0.7563169586,4.0355911855

H,0,3.1116230317,0.0469206332,3.3980160653

H,0,2.8509945775,1.7903852223,3.3021917217

H,0,3.4439473075,-0.1005419152,0.9170983671

H,0,2.1845485674,0.418824218,-0.224407518

H,0,3.1769712132,1.6208513524,0.5995135561

H,0,-0.2119148787,0.3713830822,2.681936853

H,0,0.1364292158,0.4748242114,-0.3965758553

H,0,-1.4237627425,0.368832496,0.5547096443

H,0,-2.178911237,2.5798942817,1.6344185509

H,0,-2.1001930739,4.0152248468,0.5691106878

H,0,-2.4407441295,2.3968739929,-0.1089438713

H,0,-0.8637136661,2.3171758577,-1.5838230708

H,0,-0.2437161373,3.9660073837,-1.264961829

H,0,0.8740836123,2.5844294803,-1.2257433711

H,0,0.6576519869,3.7474978296,3.4435048025

H,0,-0.9259748958,4.2368697818,2.8262334456

H,0,-0.5835949805,2.5307228666,3.1347059426

O,0,2.356286745,3.5912578344,-0.0113876941

O,0,2.4102155184,4.1551450306,2.171099764

C,0,3.7562223264,4.5260294056,1.948521487

H,0,4.1060248817,4.9696816008,2.8848148825

H,0,4.3796762012,3.6560283543,1.7027213343

H,0,3.8465439371,5.2560500083,1.1355191369

TS23/ B3LYP-D2/6-31G*/exo-cis/ PCM

/home/bibaswanbiswas/c11/exocistsB3D2SB

2,3-rearrangement looking at effect of B3D3

freq=hpmodes

E(RB3LYP) = -636.982869586

Zero-point correction= 0.308691 (Hartree/Particle)

Thermal correction to Energy= 0.325316

Thermal correction to Enthalpy= 0.326260

Thermal correction to Gibbs Free Energy= 0.266139

Sum of electronic and ZPE= -636.674178

Sum of electronic and thermal Energies= -636.657554

Sum of electronic and thermal Enthalpies= -636.656610

Sum of electronic and thermal Free Energies= -636.716730

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	204.139	62.583	126.535

C,0,-0.0899092224,0.6691163789,0.2394521644

C,0,0.3590730144,0.4114130625,1.5502554545

C,0,1.624665994,0.6901420473,2.0019436078

C,0,2.8445240202,0.7554358233,1.1267465305

C,0,1.910499675,0.7605568769,3.4753937631

N,0,-0.4517482639,2.732391293,0.4098857455

C,0,-1.8530156894,2.706364318,0.8805075589

C,0,0.4566105365,3.3153454917,1.3096259337

C,0,0.0095396691,3.5351444895,2.7349079741

C,0,1.7952203232,3.5684918424,0.8962645745

C,0,-0.4270707426,3.1606213827,-1.0095753923

H,0,1.0074471304,0.6126458524,4.0780098366

H,0,2.6625663928,0.0152357574,3.7761597363

H,0,2.3308785859,1.7489803633,3.7134285245

H,0,3.3839949715,-0.2030418609,1.1871015002

H,0,2.6190559919,0.9697064277,0.0813175516

H,0,3.5290613952,1.5331551567,1.4846398624

H,0,-0.408542523,0.2360416655,2.3048740986

H,0,0.6278477838,0.7592669375,-0.5694608412

H,0,-1.0865913183,0.3574853721,-0.0601771234

H,0,-1.9214927372,2.163945885,1.8230883763

H,0,-2.2245652777,3.7292628295,1.0127159468

H,0,-2.456619418,2.1942752554,0.1288092697

H,0,-1.0471180414,2.4653880551,-1.5822174276

H,0,-0.843357424,4.1736229216,-1.086812538

H,0,0.5991929631,3.1500737307,-1.3636446224

H,0,0.8325102737,3.9545978839,3.3128123529

H,0,-0.8394296059,4.2306149053,2.8057279345

H,0,-0.2971260965,2.6019025981,3.2273159173

O,0,2.3058263343,3.402040553,-0.2260917421

O,0,2.5844883925,4.0614875421,1.928132907

C,0,3.9123417646,4.4244593276,1.5488406292

H,0,4.3889006972,4.7903893016,2.461923405

H,0,4.4636805187,3.5640387447,1.1550342072

H,0,3.9050589327,5.2125627888,0.7866383236

TS23/ MPW1KSCF/6-31G*/ endo s-cis /PCM

/home/bibaswanbiswas/c11/me3alaMPW1KSBSCF

endo s-cis isomer of trimethylalanine system

mpwpw91/6-31G(d)

E(RmPW+HF-PW91) = -636.737347303

Zero-point correction= 0.318063 (Hartree/Particle)

Thermal correction to Energy= 0.334605

Thermal correction to Enthalpy= 0.335550

Thermal correction to Gibbs Free Energy= 0.275616

Sum of electronic and ZPE= -636.419284

Sum of electronic and thermal Energies= -636.402742

Sum of electronic and thermal Enthalpies= -636.401798

Sum of electronic and thermal Free Energies= -636.461731

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	209.968	61.469	126.140

C,0,-0.3918180362,0.5312768287,0.5587274461

C,0,0.3240129352,0.4098914181,1.741119056

C,0,1.6605225566,0.70673373,1.8595892442

C,0,2.6175916743,0.6257694082,0.716396911

C,0,2.2873978926,0.8344045786,3.2098651689

N,0,-0.3998350809,2.7085603546,0.4365447837

C,0,-1.8169528023,2.9753055147,0.6678112371

C,0,0.4652676434,3.2051298295,1.3912452905

C,0,-0.0820873914,3.4020099503,2.7697475262

C,0,1.7840417176,3.637065299,1.080460137

C,0,-0.0908025586,2.8932076477,-0.9788742079

H,0,1.5420931563,0.8626693665,4.0018093174

H,0,2.9676302883,0.0020721445,3.4084032435

H,0,2.8808820068,1.7482354957,3.2703009891

H,0,3.4379030338,-0.0451559626,0.9806684563

H,0,2.153621918,0.2411990591,-0.1883962623

H,0,3.0564238835,1.5936469623,0.4683531066

H,0,-0.2467089189,0.330787715,2.6588221749

H,0,0.1018302067,0.4418457238,-0.3969880947

H,0,-1.4502244613,0.3145982527,0.5489385497

H,0,-2.1258909375,2.6200676547,1.6419473762

H,0,-2.0210002974,4.0446642646,0.5924831337

H,0,-2.3952358567,2.4527977756,-0.0869317252

H,0,-0.817651764,2.331566789,-1.5575441421

H,0,-0.160685113,3.9481280096,-1.2458466485

H,0,0.908331,2.5493786231,-1.1944965682

H,0,0.7255573266,3.5985471133,3.4631456058

H,0,-0.7825063187,4.2391713446,2.8320605537

H,0,-0.6103184727,2.5159611375,3.1220945802

O,0,2.3775041006,3.6047378861,0.0042484053

O,0,2.4218108232,4.1504261968,2.1689979699

C,0,3.7197984431,4.6445459097,1.9320212413

H,0,4.0667083919,5.0307842628,2.8846085406

H,0,4.3895855129,3.8604712772,1.5887265985

H,0,3.7096024985,5.4426594394,1.1935150053

TS23/BH AND HLYP/6-31G*/exo s-cis/PCM

/home/bibaswanbiswas/c11/obscure/exocistsBHHSB

2,3-rearrangement looking at effect of B3D3

freq=hpmodes

E(RBHandHLYP) = -636.513957631

Zero-point correction= 0.319942 (Hartree/Particle)

Thermal correction to Energy= 0.336476

Thermal correction to Enthalpy= 0.337420

Thermal correction to Gibbs Free Energy= 0.277422

Sum of electronic and ZPE= -636.194016

Sum of electronic and thermal Energies= -636.177482

Sum of electronic and thermal Enthalpies= -636.176538

Sum of electronic and thermal Free Energies= -636.236536

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	211.142	61.221	126.277

C,0,-0.3945931961,0.5040270207,0.5884458678

C,0,0.3351528964,0.4093571411,1.7647453402

C,0,1.6776786577,0.6729249805,1.8724547449

C,0,2.6279170362,0.5841433442,0.7202607674

C,0,2.3158047967,0.8120150875,3.2199003822

N,0,-0.4112232938,2.7336840072,0.4275431243

C,0,-1.8368020631,2.9957460238,0.644257516

C,0,0.4480986764,3.2483450773,1.3807286118

C,0,-0.1066406837,3.4599614236,2.7593281706

C,0,1.7785134029,3.6464180921,1.0780114478

C,0,-0.0938299443,2.8907516796,-0.9951783788

H,0,1.5778822807,0.8380254522,4.0162333855

H,0,3.003726788,-0.0119589753,3.4163656488

H,0,2.9003933996,1.7301833618,3.2706952208

H,0,3.4481169466,-0.0856092678,0.9797760504

H,0,2.156627088,0.1991473582,-0.178091241

H,0,3.0633726159,1.5501920138,0.4692503024

H,0,-0.2278338863,0.3546377465,2.685887265

H,0,0.0827978574,0.4057502242,-0.3705888215

H,0,-1.4524286018,0.3002109422,0.5986711937

H,0,-2.1497578363,2.6610661315,1.6214008043

H,0,-2.0478345264,4.0599883271,0.5444142898

H,0,-2.4042061852,2.4539278593,-0.1014644364

H,0,-0.8237252481,2.3285290179,-1.5647466815

H,0,-0.1516368386,3.9398670355,-1.2801461313

H,0,0.8985920112,2.5326758885,-1.2025744014

H,0,0.6940111199,3.670788832,3.452684485

H,0,-0.8117140105,4.2916026682,2.8068379086

H,0,-0.6320291176,2.5781832129,3.1201778966

O,0,2.3779930529,3.591919021,0.0053915707

O,0,2.42522664,4.1568597387,2.1667275107

C,0,3.7330343164,4.6400594305,1.9371097906

H,0,4.0747392878,5.0269119443,2.8892474763

H,0,4.3965610705,3.8496171868,1.6034473815

H,0,3.7344144909,5.4332119724,1.1963699379

TS23/B3LYP-D2/6-31+G/exo s-cis/PCM**

/home/bibaswanbiswas/c11/exocistsB3D2PS

2,3-rearrangement looking at effect of B3D3

freq=hpmodes

E(RB3LYP) = -637.035481289

Zero-point correction= 0.306093 (Hartree/Particle)

Thermal correction to Energy= 0.322938

Thermal correction to Enthalpy= 0.323882

Thermal correction to Gibbs Free Energy= 0.263479

Sum of electronic and ZPE= -636.729389

Sum of electronic and thermal Energies= -636.712544

Sum of electronic and thermal Enthalpies= -636.711600

Sum of electronic and thermal Free Energies= -636.772002

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	202.646	63.272	127.127

C,0,-0.067782467,0.6438793263,0.2095712575

C,0,0.3607156802,0.3948797499,1.5261344387

C,0,1.6207229041,0.6800744877,2.0019746911

C,0,2.8532063375,0.7488466238,1.1465469998

C,0,1.8782815566,0.7401670166,3.4809303081

N,0,-0.4532708928,2.7467387769,0.4128672849

C,0,-1.8487853768,2.6990181637,0.8995131042

C,0,0.4659511905,3.30526068,1.313505178

C,0,0.0283054351,3.5251015987,2.7427609974

C,0,1.798052359,3.5782948913,0.8891187955

C,0,-0.4469689442,3.186547402,-1.0032407993

H,0,0.965260334,0.5799693419,4.0633952497

H,0,2.6282603138,-0.0049995508,3.7841448227

H,0,2.2884137843,1.7266127169,3.7405967762

H,0,3.4033615291,-0.200235193,1.2381791437

H,0,2.6402657909,0.9321249762,0.0928474325

H,0,3.5225174312,1.541967314,1.497648823

H,0,-0.4167776062,0.2121544717,2.2680452211

H,0,0.6581086506,0.7707460351,-0.5862243929

H,0,-1.0659856935,0.3515189018,-0.1010319792

H,0,-1.9048570209,2.1399130947,1.8324095544

H,0,-2.2285875157,3.7156229649,1.0544006847

H,0,-2.4561437939,2.1954349386,0.1461942027

H,0,-1.0863698925,2.5046137654,-1.5691952974

H,0,-0.8520651959,4.2050639322,-1.0656413497

H,0,0.568795632,3.1653624442,-1.3850844513

H,0,0.8636203461,3.9078706009,3.3269533986

H,0,-0.7955458042,4.2482499881,2.8178886531

H,0,-0.3092629157,2.5973980732,3.2213999619

O,0,2.3013056409,3.4001017271,-0.2387834934

O,0,2.587598835,4.1003964747,1.9042618591

C,0,3.9232738132,4.4570465597,1.5291671998

H,0,4.3940824808,4.8250129141,2.4432633387

H,0,4.4699072838,3.5905708599,1.1442890431

H,0,3.9187947908,5.2418349316,0.7647673426

TS23/UM06/6-31G*/exo-trans/PCM

/home/bibaswanbiswas/c11/allme3XTM06SB

exo s-trans isomer of trimethylalanine system

um06/6-31G*

E(UM06) = -636.480877828

Zero-point correction= 0.308387 (Hartree/Particle)

Thermal correction to Energy= 0.324463

Thermal correction to Enthalpy= 0.325407

Thermal correction to Gibbs Free Energy= 0.267388

Sum of electronic and ZPE= -636.172491

Sum of electronic and thermal Energies= -636.156415

Sum of electronic and thermal Enthalpies= -636.155471

Sum of electronic and thermal Free Energies= -636.213490

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.604	62.335	122.112

C,0,0.049256444,0.8198435278,-0.0649637651

C,0,0.412715011,0.3869881749,1.2078889044

C,0,1.6156071485,0.6653828277,1.8196186631

C,0,1.7673415624,0.525457904,3.2978734618

C,0,2.9047042721,0.8774781447,1.0987802175

N,0,-0.4828817527,2.8664567848,0.5277530097

C,0,-0.5632079996,3.5601510922,-0.7676991

C,0,-1.8469035128,2.6308329414,1.0117491153

C,0,0.4148144088,3.300393913,1.5059570329

C,0,1.7703415099,3.6593460662,1.2304863105

O,0,2.1576827322,3.5183459465,-0.0787147957

C,0,3.4595201599,3.9844717934,-0.3872399571

C,0,-0.0296722588,3.4067206794,2.9341106131

O,0,2.5856845603,4.0593970093,2.0676495623

H,0,0.817395605,0.3075719489,3.8014233535

H,0,2.4873290313,-0.2656608746,3.5606160548

H,0,2.172677807,1.4619484279,3.7151214695

H,0,3.4407374243,1.7474363632,1.5088955504

H,0,3.5564333776,0.0042353434,1.2645971574

H,0,2.7905177278,1.0138330986,0.01932425

H,0,-0.3956607277,0.0323706735,1.8561710228

H,0,0.8034262383,1.1599352203,-0.774109683

H,0,-0.9060233261,0.5264053149,-0.4980760413

H,0,-1.8464230078,1.9281538239,1.8482038109

H,0,-2.3134743456,3.5737103199,1.3315004311

H,0,-2.4410525323,2.2068494167,0.1969963304

H,0,-1.1555940702,2.9447921862,-1.4544659531

H,0,-1.0646644432,4.5306927805,-0.6354406863

H,0,0.428656556,3.7154606323,-1.1823187872

H,0,0.8076479774,3.7931588803,3.5208902611

H,0,-0.8749715114,4.0986322591,3.069624372

H,0,-0.3285194967,2.4468803643,3.3825940638

H,0,3.5755537122,3.8585804929,-1.4668729828

H,0,3.5760169926,5.0418078738,-0.1224748526

H,0,4.2329297262,3.4076716486,0.133137586

TSCleavageA/UM062X/6-31+G/PCM**

/home/bibaswanbiswas/c11/cleavageAM062XPS

trimethyl pure cleavage conf A

UM062X/6-31+G**

E(UM062X) = -636.657086476

Zero-point correction= 0.307011 (Hartree/Particle)

Thermal correction to Energy= 0.324770

Thermal correction to Enthalpy= 0.325714

Thermal correction to Gibbs Free Energy= 0.260977

Sum of electronic and ZPE= -636.350075

Sum of electronic and thermal Energies= -636.332316

Sum of electronic and thermal Enthalpies= -636.331372

Sum of electronic and thermal Free Energies= -636.396109

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.796	64.043	136.250

C,0,0.9553871407,0.0689996306,-1.0727349545

C,0,2.2372577473,-0.5260308032,-1.0216998846

C,0,3.4055144541,0.0462303844,-0.5822540643

C,0,3.5255356054,1.4743935779,-0.1354349497

C,0,4.680368427,-0.7449695972,-0.5371336616

N,0,-0.1696421495,-0.2682691109,0.8479627406

C,0,0.7710958592,0.3547099394,1.7823746669

C,0,-1.4100220561,0.333004453,0.7122904676

C,0,-1.6220331827,1.7051102716,1.288579426

C,0,-2.3413561651,-0.2206046386,-0.2217171913

C,0,-0.0869258022,-1.7344823517,0.951629873

H,0,4.5315338329,-1.7754676656,-0.8687116222

H,0,5.4487081155,-0.2840780463,-1.1710704882

H,0,5.0897442951,-0.763971888,0.4812711394

H,0,4.3046567352,1.9863649319,-0.7138371237

H,0,2.5984150868,2.0403468539,-0.2390406641

H,0,3.8372531277,1.5216072973,0.9163628406

H,0,2.2944955413,-1.5716767215,-1.326286438

H,0,0.8253083783,1.1371093582,-0.9290647205

H,0,0.1481241753,-0.445011923,-1.5825839198

H,0,0.8373890196,1.4269833304,1.6059927269

H,0,0.4576601057,0.1711540714,2.8175746427

H,0,1.753497885,-0.0928680326,1.6187258458

H,0,0.9574682058,-2.0244642834,0.8213833187

H,0,-0.4275289074,-2.03879509,1.9490130828

H,0,-0.7020560658,-2.1970309813,0.1866198681

H,0,-2.6656842223,1.9905244221,1.1726334862

H,0,-1.3744788508,1.7477116988,2.3539069001

H,0,-1.0137946473,2.4680757583,0.7804463934

O,0,-2.1689841428,-1.1972231614,-0.9652771375

O,0,-3.5270598947,0.4631247539,-0.2575475515

C,0,-4.4848927476,-0.0197071962,-1.1934632127

H,0,-5.3440931836,0.6441981211,-1.1051399094

H,0,-4.0861842686,0.0123650608,-2.2102485469

H,0,-4.7772464512,-1.0459774238,-0.9580353784

Polyrate Structures for Rearrangement of Alanineprenyl Ammonium Salt B3LYP-D2/6-31+G/PCM**

23 Starting Material

pb3lypd2/geom/sm/ g091.log

sm for 23 from opt of ts

B3LYP/6-31+G**

E(RB3LYP) = -637.056800173

Zero-point correction= 0.309833 (Hartree/Particle)

Thermal correction to Energy= 0.326548

Thermal correction to Enthalpy= 0.327492

Thermal correction to Gibbs Free Energy= 0.266676

Sum of electronic and zero-point Energies= -636.746968

Sum of electronic and thermal Energies= -636.730252

Sum of electronic and thermal Enthalpies= -636.729308

Sum of electronic and thermal Free Energies= -636.790124

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	204.912	62.890	127.999

C,0,1.4846763454,0.9475808171,-1.3323944738

C,0,1.0457625478,2.0602645145,-0.4362992417

C,0,-0.2247591393,2.4277829553,-0.1911145892

C,0,-1.4472766018,1.7870875597,-0.7923237938

C,0,-0.5201024856,3.5460217453,0.7761402919

N,0,1.7647051994,-0.367360139,-0.5598126214

C,0,2.848375725,-0.1025848522,0.445098352

C,0,0.5235136685,-0.9018982347,0.1044084261

C,0,0.3683447106,-0.656214674,1.5825758622

C,0,-0.5191519974,-1.2615102035,-0.7406196032

C,0,2.3394193708,-1.3613127071,-1.5407037273

H,0,0.3941822551,3.9790982931,1.1949080609

H,0,-1.096894036,4.3402983594,0.2831778995

H,0,-1.142238737,3.1720078837,1.6015184845

H,0,-2.1274267716,2.563885481,-1.1664475318

H,0,-1.2222015308,1.0868409173,-1.5974443973

H,0,-1.9888294007,1.2319358135,-0.0143804201

H,0,1.8389051845,2.6043487301,0.0731422918

H,0,0.737963203,0.667662139,-2.0733689619

H,0,2.4244942817,1.1968764731,-1.8353505011

H,0,2.5083843399,0.6365641997,1.1659558884

H,0,3.0877279077,-1.0393238184,0.9480190634

H,0,3.7180255391,0.2734945894,-0.0963296101

H,0,3.2386745346,-0.9270640938,-1.9848747274

H,0,2.5822976972,-2.2667808203,-0.9835708845

H,0,1.5817069385,-1.5635650896,-2.2936442408

H,0,-0.5853680967,-1.0817825015,1.8986633081

H,0,1.1510071235,-1.1257220057,2.1939972652

H,0,0.351282542,0.4157013795,1.83900044

O,0,-0.5435163311,-1.2804192408,-2.0051325647

O,0,-1.6798845343,-1.6404121468,-0.0485799211

C,0,-2.8105480152,-1.9478775344,-0.8648925241

H,0,-3.6138192188,-2.2031725664,-0.1687135202

H,0,-3.1047606153,-1.0861055233,-1.4747640023

H,0,-2.6084466028,-2.7963906992,-1.5283197762

23 Product

pb3lypd2/geom/p/g091.log

B3LYP/6-31+G**

E(RB3LYP) = -637.085989816

Zero-point correction= 0.309693 (Hartree/Particle)

Thermal correction to Energy= 0.326159

Thermal correction to Enthalpy= 0.327103

Thermal correction to Gibbs Free Energy= 0.267762

Sum of electronic and zero-point Energies= -636.776297

Sum of electronic and thermal Energies= -636.759831

Sum of electronic and thermal Enthalpies= -636.758886

Sum of electronic and thermal Free Energies= -636.818228

C,0,1.9035878192,2.2318895432,-1.3352584808

C,0,1.2449339646,2.0374675082,-0.1893731577

C,0,-0.1731308191,1.5229975942,-0.0275924204

C,0,-0.8041345181,1.0067820133,-1.3405003258

C,0,-1.0092886502,2.7730391766,0.3679617463

N,0,1.0430854135,-0.4450273805,1.0425955787

C,0,1.2085964292,-1.4004733754,2.1471599109

C,0,-0.1689028241,0.4017785246,1.1288270414

C,0,-0.1838756322,1.079341469,2.5219794608

C,0,-1.4648630119,-0.4420071879,1.0044078342

C,0,1.3340234945,-1.0991575591,-0.2401649416

H,0,-0.5496730281,3.3326721591,1.1874429526

H,0,-1.059504702,3.4344167836,-0.5031926586

H,0,-2.0253837588,2.4911677198,0.6562919954

H,0,-0.6991226504,1.7701273814,-2.1175341427

H,0,-0.3682649598,0.0780097981,-1.7083132666

H,0,-1.8767882093,0.8442244457,-1.1904020908

H,0,1.7212408331,2.3243970359,0.7461683297

H,0,1.4814279079,1.9565120224,-2.298283643

H,0,2.9000549061,2.6660246969,-1.3381228467

H,0,1.3255586724,-0.8849565082,3.1025913062

H,0,0.374613001,-2.1171077192,2.2276797579

H,0,2.1277643003,-1.9676155356,1.9722208929

H,0,1.4969522051,-0.3556131354,-1.0183328243

H,0,2.2721820469,-1.6525584936,-0.1262808043

H,0,0.5521124808,-1.8031337877,-0.55902938

H,0,-1.0200389923,1.7696126979,2.6084969712

H,0,-0.2944550608,0.3414320301,3.318813033

H,0,0.7556429266,1.6192404475,2.6712512993

O,0,-1.5183570476,-1.6074534412,0.6525010617

O,0,-2.5658689681,0.2622691655,1.3321484324

C,0,-3.8315611563,-0.4246968558,1.2009819499

H,0,-4.5873925296,0.3038284828,1.4944659991

H,0,-3.9783041027,-0.7426072462,0.1650046021

H,0,-3.8543787796,-1.2968224698,1.8596808277

23 Transition State

pb3lypd2/geom/ts/ g091.log

alanine prenyl TSfreq

B3LYP/6-31+G**

E(RB3LYP) = -637.038443161

Zero-point correction= 0.306141 (Hartree/Particle)

Thermal correction to Energy= 0.322963

Thermal correction to Enthalpy= 0.323907

Thermal correction to Gibbs Free Energy= 0.263544

Sum of electronic and zero-point Energies= -636.732302

Sum of electronic and thermal Energies= -636.715480

Sum of electronic and thermal Enthalpies= -636.714536

Sum of electronic and thermal Free Energies= -636.774900

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	202.662	63.207	127.046

C,0,-0.0711494365,0.6534223104,0.2120586619

C,0,0.3595368194,0.4000549812,1.5285831057

C,0,1.6196556726,0.6842974269,2.0019265126

C,0,2.8513470929,0.7559656259,1.1455036

C,0,1.8789860945,0.7506965606,3.4799959512

N,0,-0.4528476097,2.7418043194,0.411096931

C,0,-1.8488283417,2.6996356121,0.898461198

C,0,0.4660189769,3.3047588665,1.3114069961

C,0,0.0298750619,3.5121485453,2.7430267345

C,0,1.7974245305,3.5774569654,0.8876441811

C,0,-0.4459486683,3.1811858806,-1.0055674053

H,0,0.9679817991,0.5867040981,4.0647677797

H,0,2.6351962351,0.0127604754,3.7851837328

H,0,2.2815861882,1.7419948628,3.7328745375

H,0,3.4068761238,-0.1894547678,1.2417036216

H,0,2.6367034935,0.9336315729,0.0913102846

H,0,3.5153034605,1.5551989341,1.4930524807

H,0,-0.4173153709,0.220517796,2.2718030331

H,0,0.6544450008,0.7732114235,-0.5855002641

H,0,-1.0689614779,0.3582940612,-0.0978809993

H,0,-1.9074218015,2.1344438237,1.827570635

H,0,-2.2213214054,3.7176260342,1.0605961552

H,0,-2.4597832037,2.2049092123,0.1422905692

H,0,-1.0920806912,2.5039135035,-1.5694695513

H,0,-0.842286767,4.2030342238,-1.0673997637

H,0,0.5691744301,3.1512301523,-1.3886168593

H,0,0.8664122524,3.8868531585,3.3308078059

H,0,-0.7931185344,4.235474489,2.8265066651

H,0,-0.3084542661,2.5788808935,3.2101309294

O,0,2.3011075583,3.4036560171,-0.2409739939

O,0,2.5882896464,4.093225861,1.9055303063

C,0,3.9241808282,4.4500013951,1.5321242688

H,0,4.3941583104,4.8161548947,2.4474763248

H,0,4.4709082461,3.5837085426,1.1469095366

H,0,3.9207487529,5.2357632482,0.7686402981

Polyrate Structures for Rearrangement of Alanineprenyl Ammonium Salt M06/6-31+G/PCM**

23 Starting Material

pm06only23/geom/sm/alanineprenyl23smm06631plusgstarstarpcm

sm for 23 from opt of ts

M06/6-31+G**

E(RM06) = -636.554189139

Zero-point correction= 0.308245 (Hartree/Particle)

Thermal correction to Energy= 0.325010

Thermal correction to Enthalpy= 0.325954

Thermal correction to Gibbs Free Energy= 0.265694

Sum of electronic and ZPE= -636.245944

Sum of electronic and thermal Energies= -636.229179

Sum of electronic and thermal Enthalpies= -636.228235

Sum of electronic and thermal Free Energies= -636.288495

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.947	63.374	126.827

C,0,1.4534289807,0.9419096635,-1.3197179856

C,0,1.0429666568,2.0639055153,-0.4355663187

C,0,-0.2139456443,2.4742702393,-0.1964388234

C,0,-1.4513208212,1.8650120562,-0.776306911

C,0,-0.4714327515,3.6091480972,0.7461992758

N,0,1.7462703963,-0.3634412715,-0.5535198845

C,0,2.8220278385,-0.0966405521,0.4438821289

C,0,0.5188693013,-0.9233259722,0.1118183056

C,0,0.3563125672,-0.7247349551,1.5871005339

C,0,-0.5187699018,-1.2813682105,-0.7417175141

C,0,2.3256104103,-1.344456203,-1.5308997444

H,0,0.4537136084,4.0338988143,1.1486946586

H,0,-1.0382898198,4.4096782028,0.2524705456

H,0,-1.0897042019,3.2670403193,1.5884915059

H,0,-2.0864022917,2.6452636719,-1.2166530956

H,0,-1.2597800256,1.0969303211,-1.5308070177

H,0,-2.0423738811,1.3996613499,0.0267970918

H,0,1.8516713926,2.6061735746,0.0590452313

H,0,0.6917750011,0.6616666854,-2.0511855552

H,0,2.3817300291,1.183639628,-1.8532728959

H,0,2.4747494583,0.6078786615,1.198222343

H,0,3.1039328485,-1.0390257674,0.9176801029

H,0,3.6808932695,0.3240207582,-0.0855386197

H,0,3.2300727709,-0.9150334106,-1.9722389898

H,0,2.5668454725,-2.2568152203,-0.9817605049

H,0,1.5767444291,-1.5507479018,-2.2941858192

H,0,-0.5806765725,-1.2014784962,1.8837913364

H,0,1.1455580777,-1.1843051632,2.198308938

H,0,0.2823437136,0.3341748265,1.8939375228

O,0,-0.5432664496,-1.2730445263,-1.9963889037

O,0,-1.6602459666,-1.6943857044,-0.0606645297

C,0,-2.7713506708,-2.0204347761,-0.8724749572

H,0,-3.5696646089,-2.3159231682,-0.1872098435

H,0,-3.103044588,-1.1610666861,-1.4683854083

H,0,-2.551023027,-2.8500894,-1.5539821986

23 Product

pm06only23/geom/p/alanineprenyl23pdtm06631plusgstarstarpcm

23 product

M06/6-31+G**

E(RM06) = -636.584166461

Zero-point correction= 0.307900 (Hartree/Particle)

Thermal correction to Energy= 0.324587

Thermal correction to Enthalpy= 0.325531

Thermal correction to Gibbs Free Energy= 0.265848

Sum of electronic and ZPE= -636.276266

Sum of electronic and thermal Energies= -636.259580

Sum of electronic and thermal Enthalpies= -636.258636

Sum of electronic and thermal Free Energies= -636.318318

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.681	63.899	125.613

C,0,1.8862740754,2.233417533,-1.347090206

C,0,1.239496733,2.0216864595,-0.2013407867

C,0,-0.1752422235,1.5180726303,-0.0263320537

C,0,-0.8096444633,1.0094071305,-1.3284553596

C,0,-0.989157259,2.7699326929,0.3665041454

N,0,1.0225774361,-0.4470130149,1.0442833738

C,0,1.189209052,-1.3819110438,2.1507891388

C,0,-0.1778062177,0.4070728857,1.1235674078

C,0,-0.1936549231,1.0675006112,2.5111294614

C,0,-1.4657851323,-0.4268687777,0.9836030017

C,0,1.3426992311,-1.1125875348,-0.2137721759

H,0,-0.5218688213,3.338339189,1.1773740068

H,0,-1.0376659883,3.4321589383,-0.5059784108

H,0,-2.0136228342,2.5163142552,0.6597576825

H,0,-0.7254395543,1.7753601375,-2.1076133005

H,0,-0.3718238286,0.0860194701,-1.7151199169

H,0,-1.8833748254,0.833350682,-1.1837852118

H,0,1.7323674079,2.3046620836,0.7316672157

H,0,1.4644744005,1.9739319549,-2.3169419538

H,0,2.8819174047,2.6703880176,-1.353372385

H,0,1.3028365264,-0.8664189959,3.1078819676

H,0,0.364545842,-2.1121740459,2.2393117812

H,0,2.1119257615,-1.947571877,1.9865532802

H,0,1.4458939425,-0.3941291613,-1.0279365781

H,0,2.3226436269,-1.5899133764,-0.0985119383

H,0,0.6165433993,-1.8888381853,-0.5028333398

H,0,-1.0046860678,1.7882943259,2.6042357405

H,0,-0.3451750113,0.328325238,3.3024610337

H,0,0.7602013159,1.5739355443,2.6965222477

O,0,-1.5269976856,-1.5609389981,0.556555661

O,0,-2.5546052985,0.2471588766,1.3829486337

C,0,-3.8077407687,-0.4235081904,1.2096490386

H,0,-4.5685842756,0.2659907175,1.5743010901

H,0,-3.9738432954,-0.6485912284,0.1514796817

H,0,-3.8284006812,-1.3528549433,1.7847980271

23 Transition State

pm06only23/geom/ts/alanineprenyl23tsm06631plusgstarstarpcm

alanine prenyl TSfreq

M06/6-31+G**

E(RM06) = -636.529717334

Zero-point correction= 0.303801 (Hartree/Particle)

Thermal correction to Energy= 0.321062

Thermal correction to Enthalpy= 0.322006

Thermal correction to Gibbs Free Energy= 0.260154

Sum of electronic and ZPE= -636.225916

Sum of electronic and thermal Energies= -636.208655

Sum of electronic and thermal Enthalpies= -636.207711

Sum of electronic and thermal Free Energies= -636.269563

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	201.469	64.166	130.179

C,0,-0.0967635102,0.5733433215,0.2479843634

C,0,0.3560741693,0.3734367964,1.552212669

C,0,1.6271619764,0.6628581776,1.9994840886

C,0,2.8288262866,0.7116961137,1.1151795494

C,0,1.9270550387,0.6812857028,3.4625831317

N,0,-0.4441797728,2.7513925886,0.4228822161

C,0,-1.8419709342,2.7486209027,0.8708871376

C,0,0.4693372423,3.2872262733,1.3313657656

C,0,0.0209606377,3.5563301171,2.7383390102

C,0,1.8005761836,3.583661651,0.9113156818

C,0,-0.3944807243,3.1583022193,-0.9915825953

H,0,1.0311544896,0.533191449,4.0750442098

H,0,2.6585994743,-0.0975743827,3.725229657

H,0,2.3853506673,1.6399315175,3.7480793153

H,0,3.3279352015,-0.2694525631,1.129354306

H,0,2.6062761683,0.9712741117,0.0773851763

H,0,3.5606938321,1.4401167785,1.4879420422

H,0,-0.4038469289,0.1883770631,2.3166906055

H,0,0.6047845178,0.6883705706,-0.575644125

H,0,-1.1089370139,0.2898303092,-0.0321680433

H,0,-1.9545243519,2.208974511,1.8124759563

H,0,-2.2082687216,3.7770990726,0.9966249432

H,0,-2.4515393668,2.2516809902,0.112761705

H,0,-1.0605137778,2.5033309633,-1.5612484484

H,0,-0.7442843618,4.1966070351,-1.087685474

H,0,0.6210010449,3.081536116,-1.3713252802

H,0,0.8727329636,3.8653947133,3.3446203297

H,0,-0.7315811049,4.3566243771,2.7989253741

H,0,-0.4149853967,2.6728773322,3.2234977508

O,0,2.3167817448,3.3878343672,-0.1978729349

O,0,2.5514315935,4.1610793458,1.9105448389

C,0,3.8667734619,4.5487486919,1.5459657395

H,0,4.3127473105,4.9779752546,2.4452605227

H,0,4.4628339179,3.6928666325,1.2115310368

H,0,3.8531870433,5.2983128795,0.7469337784

Polyrate Structures for Rearrangement of Alanineprenyl Ammonium salt

M062X/6-31+G/PCM**

23 Starting Material

pm0623/geom/sm/alanineprenyl23smm062x631plusgstarstarpcm

sm for 23 from opt of ts

m062x/6-31+G**

E(RM062X) = -636.700911132

Zero-point correction= 0.313391 (Hartree/Particle)

Thermal correction to Energy= 0.330063

Thermal correction to Enthalpy= 0.331007

Thermal correction to Gibbs Free Energy= 0.270419

Sum of electronic and ZPE= -636.387521

Sum of electronic and thermal Energies= -636.370848

Sum of electronic and thermal Enthalpies= -636.369904

Sum of electronic and thermal Free Energies= -636.430493

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	207.118	62.441	127.519

C,0,1.4584992874,0.9297615226,-1.3432165067

C,0,1.0565837422,2.0684336546,-0.4593737405

C,0,-0.2006833018,2.4436681586,-0.1781096807

C,0,-1.4420819195,1.7723778809,-0.6991304425

C,0,-0.4606140274,3.5974123671,0.7537525743

N,0,1.7456763513,-0.3581883775,-0.5615850793

C,0,2.8104173671,-0.0777779167,0.4482418744

C,0,0.5098562453,-0.8944585761,0.0979998108

C,0,0.3309932941,-0.674052431,1.5734403763

C,0,-0.5166636392,-1.2675725626,-0.7544943714

C,0,2.3290134829,-1.358499082,-1.5195196147

H,0,0.465734649,4.0379121925,1.1290432174

H,0,-1.0423258903,4.3764701589,0.2485994891

H,0,-1.05889224,3.2600459748,1.6086057497

H,0,-2.1592860365,2.5272476796,-1.039546008

H,0,-1.2506476944,1.0695481985,-1.5112778009

H,0,-1.9220006793,1.2134763837,0.1149978673

H,0,1.8694781028,2.6385361226,-0.0121441787

H,0,0.6893363935,0.6495311282,-2.062511619

H,0,2.3819118076,1.1672090256,-1.8805315995

H,0,2.4481151869,0.6399242145,1.1796216073

H,0,3.0771292083,-1.0127806729,0.9397548074

H,0,3.6745062349,0.3300155122,-0.0777700457

H,0,3.2435035681,-0.9412134019,-1.9452830155

H,0,2.5495210854,-2.2636595293,-0.9549430465

H,0,1.5915565207,-1.5611459456,-2.2909462229

H,0,-0.6123692625,-1.1372943806,1.8620974181

H,0,1.1124157809,-1.1302896037,2.1920603868

H,0,0.2681146803,0.3899070152,1.8514308385

O,0,-0.5284621147,-1.2802995016,-2.0139974213

O,0,-1.6690787466,-1.662932635,-0.0831250787

C,0,-2.7770591758,-1.978308216,-0.9105307161

H,0,-3.5864536047,-2.2488762365,-0.2314314983

H,0,-3.0756258373,-1.1184316956,-1.5175387227

H,0,-2.5558938186,-2.8177414253,-1.5751156078

23 Product

pm0623/geom/p/alanineprenyl23pdtm062x631plusgstarstarpcm

23 product

m062x/6-31+G**

E(RM062X) = -636.730284009

Zero-point correction= 0.312703 (Hartree/Particle)

Thermal correction to Energy= 0.329204

Thermal correction to Enthalpy= 0.330148

Thermal correction to Gibbs Free Energy= 0.270955

Sum of electronic and ZPE= -636.417581

Sum of electronic and thermal Energies= -636.401080

Sum of electronic and thermal Enthalpies= -636.400136

Sum of electronic and thermal Free Energies= -636.459329

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 206.579 63.125 124.582

C,0,1.8793957426,2.2109073683,-1.3632725251

C,0,1.2451660138,2.0222859089,-0.2062587707

C,0,-0.1744416023,1.5244843344,-0.0155512312

C,0,-0.8269192102,1.016692385,-1.3148692872

C,0,-0.9845996273,2.778273967,0.3975885675

N,0,1.0422827026,-0.4332982717,1.0452480794

C,0,1.2096509049,-1.3679896982,2.1589564865

C,0,-0.1649232701,0.4074503646,1.1295332952

C,0,-0.2006912837,1.0613740392,2.526045063

C,0,-1.4511831555,-0.4358696637,0.9905341751

C,0,1.3247677124,-1.1060415274,-0.22386756

H,0,-0.5060081909,3.3291135707,1.2107887532

H,0,-1.0376789884,3.4465142795,-0.4667274507

H,0,-2.0026947556,2.5165932654,0.6969343434

H,0,-0.7463436921,1.7812493413,-2.0922933883

H,0,-0.396203816,0.0917677027,-1.6997435977

H,0,-1.8960564339,0.8474701341,-1.1486240492

H,0,1.7491435251,2.3073767014,0.7171671248

H,0,1.4400258188,1.940773313,-2.3196845153

H,0,2.8782501987,2.6352129972,-1.3854293495

H,0,1.3701527903,-0.839687671,3.0994517959

H,0,0.3613871926,-2.0603480238,2.2785398863

H,0,2.1045088847,-1.9643582683,1.9694115174

H,0,1.4502330652,-0.3801190381,-1.0243689899

H,0,2.2818199442,-1.6234537665,-0.1158226054

H,0,0.5634077608,-1.8433188691,-0.5110449097

H,0,-1.0355957598,1.7522783099,2.6122551162

H,0,-0.3269872533,0.3113380823,3.3083863368

H,0,0.7356488589,1.5967428753,2.707843191

O,0,-1.5003102381,-1.5937072146,0.6347436242

O,0,-2.5514756569,0.2609564815,1.3095006626

C,0,-3.799267196,-0.4277868202,1.1538012298

H,0,-4.5672497288,0.2860987939,1.4431433981

H,0,-3.9312980654,-0.7343494467,0.1140591804

H,0,-3.8274261908,-1.3066259359,1.7999164029

23 Transition State

pm0623/geom/ts/alanineprenyl23tsm062x631plusgstarstarpcm

alanine prenyl TSfreq

M062x/6-31+G**

E(RM062X) = -636.669052060

Zero-point correction= 0.310285 (Hartree/Particle)

Thermal correction to Energy= 0.326670

Thermal correction to Enthalpy= 0.327615

Thermal correction to Gibbs Free Energy= 0.268567

Sum of electronic and ZPE= -636.358767

Sum of electronic and thermal Energies= -636.342382

Sum of electronic and thermal Enthalpies= -636.341437

Sum of electronic and thermal Free Energies= -636.400486

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	204.989	62.372	124.277

C,0,-0.3044454378,0.5661859359,0.4335824281

C,0,0.3117070217,0.3894461711,1.6811629742

C,0,1.6116351182,0.7763004301,1.9270903852

C,0,2.6882809513,0.7876243167,0.8773580043

C,0,2.1219511777,0.88649285,3.3355380128

N,0,-0.4136766219,2.6604975751,0.4198765702

C,0,-1.8382639263,2.8704440583,0.7486704839

C,0,0.483607709,3.167439842,1.3637646054

C,0,-0.0201257197,3.3687612474,2.7689201608

C,0,1.7928178691,3.6047609818,0.9919245768

C,0,-0.1984724756,2.9417328411,-1.0150623904

H,0,1.3182693163,0.7939336764,4.0707859205

H,0,2.8742268936,0.1135814489,3.5406858696

H,0,2.6139308949,1.8581500383,3.4736228624

H,0,3.2063150443,-0.1807690251,0.8923677239

H,0,2.3173662872,0.9661143392,-0.132715371

H,0,3.4366635888,1.5570140534,1.092420703

H,0,-0.3383874594,0.2416296319,2.5431596604

H,0,0.284263686,0.5217756267,-0.4772626086

H,0,-1.3510310405,0.2994486557,0.3122485987

H,0,-2.0781915856,2.4285025666,1.7135667978

H,0,-2.0653298007,3.9421695306,0.7667169675

H,0,-2.4431591263,2.3861194528,-0.0174365824

H,0,-0.9642323262,2.4016190967,-1.5739695932

H,0,-0.2958943917,4.0163700031,-1.2025530266

H,0,0.7893390956,2.6169755359,-1.3213775655

H,0,0.8137351208,3.5971432272,3.4292943686

H,0,-0.7434299329,4.1911643969,2.8439915005

H,0,-0.5095631473,2.4681437101,3.1557873576

O,0,2.3227106271,3.6146093617,-0.1261554295

O,0,2.5127410336,4.056301066,2.0730766297

C,0,3.8183986158,4.5409621723,1.7817306646

H,0,4.2347043411,4.8569636685,2.737757578

H,0,4.4418154424,3.7579465512,1.3429413878

H,0,3.7761221576,5.3876059654,1.0920637746

Polyrate structures for C-N Bond Cleavage in Alanineprenyl Ammonium salt

B3LYP-D2/6-31+G/PCM**

Cleavage A Starting Material

SM_Ylide_Cleavage/ Ab3lyp_d2ps1.log

SM Alanine ammonium dimethyl allyl ylide

b3lyp/6-31+g**

E(RB3LYP) = -637.054742510

Zero-point correction= 0.309431 (Hartree/Particle)

Thermal correction to Energy= 0.326397

Thermal correction to Enthalpy= 0.327341

Thermal correction to Gibbs Free Energy= 0.265483

Sum of electronic and zero-point Energies= -636.745311

Sum of electronic and thermal Energies= -636.728346

Sum of electronic and thermal Enthalpies= -636.727402

Sum of electronic and thermal Free Energies= -636.789260

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	204.817	63.124	130.191

C,0,0.7503973531,-0.4733121616,-0.4453787405

C,0,2.1318469562,-0.9407591219,-0.1076912437

C,0,3.2843811244,-0.3267548752,-0.4343809345

C,0,3.3869605786,0.9760597734,-1.1839345861

C,0,4.6118493423,-0.9218399061,-0.0390324679

N,0,0.0289885937,0.2999389941,0.6884557427

C,0,0.8427313192,1.5122023897,1.0400427685

C,0,-1.3485546938,0.6997944273,0.2258757009

C,0,-1.4587041714,2.0570952452,-0.42231885

C,0,-2.2441240671,-0.3423021669,-0.0224220165

C,0,-0.0186275443,-0.5458867826,1.9365493365

H,0,4.4897314779,-1.8564353559,0.5176654141

H,0,5.2238662363,-1.1175752372,-0.9300014816

H,0,5.1767807272,-0.2120644294,0.580989555

H,0,4.0601319639,0.8621225465,-2.0433324321

H,0,2.4274498431,1.353308131,-1.542855851

H,0,3.8323755734,1.7416059292,-0.5335266446

H,0,2.1928729832,-1.8740784843,0.4486334364

H,0,0.727487572,0.2128494372,-1.2926828738

H,0,0.0876363181,-1.3160741382,-0.6439470937

H,0,0.9855371016,2.1257406023,0.1537546884

H,0,0.3039837063,2.0696661419,1.8063375204

H,0,1.8078670429,1.1722492022,1.4132542874

H,0,1.0060903669,-0.772818508,2.236506999

H,0,-0.5254678037,0.0410978972,2.7034178655

H,0,-0.580168279,-1.4483441119,1.710778516

H,0,-2.4762527901,2.1763230571,-0.7973497801

H,0,-1.260284765,2.8928045247,0.2615719055

H,0,-0.7798321168,2.1813406291,-1.2856733467

O,0,-2.1048649723,-1.5763066919,0.2035860696

O,0,-3.4501707154,0.0993812151,-0.5849043899

C,0,-4.4462004625,-0.9064304642,-0.782703749

H,0,-5.2995770478,-0.3890847375,-1.2285664463

H,0,-4.0912230294,-1.6936385886,-1.4569572451

H,0,-4.7431457215,-1.3654113819,0.1675223673

Cleavage A Product

SM_Ylide_Cleavage_pdt/apps1.log

ub3lyp/6-31+g**

E(UB3LYP) = -637.032309571

Zero-point correction= 0.301659 (Hartree/Particle)

Thermal correction to Energy= 0.321232

Thermal correction to Enthalpy= 0.322176

Thermal correction to Gibbs Free Energy= 0.252304

Sum of electronic and zero-point Energies= -636.730651

Sum of electronic and thermal Energies= -636.711078

Sum of electronic and thermal Enthalpies= -636.710134

Sum of electronic and thermal Free Energies= -636.780005

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	201.576	67.836	147.057

C,0,0.7965536274,-0.7737096786,-0.802977391

C,0,2.0434101084,-1.0562752399,-0.2615785688

C,0,3.1976082271,-0.2737627921,-0.3309081377

C,0,3.2729331374,1.0329037146,-1.0680156413

C,0,4.4683278927,-0.7179542809,0.3353311074

N,0,-0.4207760186,0.7914280154,1.2544073424

C,0,0.6580310046,1.7728420202,1.2187088049

C,0,-1.6482771225,1.0889422373,0.7162269222

C,0,-1.8699969368,2.4767230654,0.1719137122

C,0,-2.615084735,0.0436312436,0.5005838827

C,0,-0.2200397985,-0.2103746453,2.3027370345

H,0,4.3445161276,-1.6761794076,0.8516328892

H,0,5.2821916673,-0.8211234411,-0.3992008855

H,0,4.809662916,0.0304010576,1.0672392749

H,0,4.0257365133,0.9774652389,-1.8688798304

H,0,2.3206086958,1.3289024728,-1.5144508764

H,0,3.5986597001,1.836968739,-0.3917028103

H,0,2.1333390298,-1.9831608276,0.3070104216

H,0,0.6056612879,0.1349348243,-1.3644790018

H,0,-0.0499380464,-1.426551871,-0.6214584821

H,0,0.6408932279,2.3387215352,0.2876833801

H,0,0.5898492674,2.4687706536,2.0687845438

H,0,1.6063243444,1.2315180637,1.2766466805

H,0,0.7400249098,-0.706782682,2.1304380783

H,0,-0.190071301,0.2924980481,3.2817482205

H,0,-1.0182983448,-0.9467430196,2.2835468625

H,0,-2.9306965642,2.6478056125,-0.0102566374

H,0,-1.3385507689,2.6300097002,-0.7799611363

H,0,-1.5055909784,3.2359697315,0.8730135476

O,0,-2.4548765837,-1.175998272,0.6855465918

O,0,-3.8144806891,0.5261821937,0.0251739017

C,0,-4.8187040762,-0.4627595298,-0.2456161426

H,0,-5.681133431,0.0928664635,-0.6181711674

H,0,-4.4678220629,-1.1745273007,-0.9998943894

H,0,-5.0811212269,-1.008311643,0.6666068997

Cleavage A Transition State

SM_Ylide_Cleavage_ts/atspcmps1.log

alanine prenyl TSfreq

UB3LYP/6-31+G**

E(UB3LYP) = -637.029145424

Zero-point correction= 0.303912 (Hartree/Particle)

Thermal correction to Energy= 0.321624

Thermal correction to Enthalpy= 0.322568

Thermal correction to Gibbs Free Energy= 0.258533

Sum of electronic and zero-point Energies= -636.725234

Sum of electronic and thermal Energies= -636.707522

Sum of electronic and thermal Enthalpies= -636.706577

Sum of electronic and thermal Free Energies= -636.770613

E (Thermal) CV S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	201.822	64.244	134.774

C,0,0.9631906469,-0.7669448014,-0.8301175942

C,0,2.243089843,-1.1128395882,-0.3491918605

C,0,3.4020765477,-0.3735932901,-0.4560786194

C,0,3.5015020738,0.9318626831,-1.1944511423

C,0,4.6830665281,-0.8565337892,0.1637080209

N,0,-0.1508335904,0.4264048875,0.7650837899

C,0,0.8080438653,1.5285070138,0.922844939

C,0,-1.4124135741,0.7452089037,0.2655972281

C,0,-1.6305689415,2.1241554927,-0.3035465377

C,0,-2.3438251887,-0.3128805367,0.0272595597

C,0,-0.0430085067,-0.4987963153,1.9114805342

H,0,4.549337182,-1.8097406188,0.6862137326

H,0,5.4639190595,-0.9828673987,-0.6014989015

H,0,5.0718717042,-0.1164680781,0.8796213648

H,0,4.2621143666,0.8619440883,-1.9858173573

H,0,2.5584725297,1.2424185431,-1.6497018098

H,0,3.8331599799,1.7306112494,-0.5151297568

H,0,2.314667627,-2.0442872225,0.2129776622

H,0,0.8253395768,0.0768056326,-1.4969838853

H,0,0.1536061511,-1.4853071054,-0.7835246323

H,0,0.8557887955,2.1292190022,0.0161137047

H,0,0.521324172,2.1628136157,1.7723212687

H,0,1.7908248497,1.0910781753,1.1097977814

H,0,0.997344259,-0.823324952,1.9878626433

H,0,-0.3297637908,0.0363721654,2.8272530757

H,0,-0.692106823,-1.3554963091,1.7543393197

H,0,-2.6798889474,2.255489729,-0.5667979158

H,0,-1.3538990658,2.9085339786,0.4112029623

H,0,-1.0353173897,2.2946948606,-1.2154832061

O,0,-2.1619422922,-1.53483807,0.2019814739

O,0,-3.5549635499,0.1395339302,-0.4600445046

C,0,-4.5299138318,-0.8735163511,-0.7414405814

H,0,-5.4025551639,-0.3397744088,-1.1230392463

H,0,-4.1555887607,-1.5770768803,-1.4924123422

H,0,-4.7903783413,-1.4269022354,0.1668838327

Polyrate Structures for C-N Bond Cleavage in Alanineprenyl Ammonium Salt

M06/6-31+G/PCM**

Cleavage A Starting Material

SM_Ylide_Cleavage/alanineprenylcleavageAsmm06631plusgstarstarpcm

SM Alanine ammonium dimethyl allyl ylide

m06/6-31+g**

E(RM06) = -636.552177221

Zero-point correction= 0.307731 (Hartree/Particle)

Thermal correction to Energy= 0.324900

Thermal correction to Enthalpy= 0.325844

Thermal correction to Gibbs Free Energy= 0.263370

Sum of electronic and ZPE= -636.244446

Sum of electronic and thermal Energies= -636.227278

Sum of electronic and thermal Enthalpies= -636.226334

Sum of electronic and thermal Free Energies= -636.288808

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.878	63.675	131.488

C,0,0.7641437801,-0.4285014282,-0.3859347284

C,0,2.1398391687,-0.8830888352,-0.0470216589

C,0,3.2921094585,-0.3282488124,-0.4621019477

C,0,3.402935776,0.8999492819,-1.3109025326

C,0,4.6090237697,-0.9277538359,-0.0763220584

N,0,0.0170227086,0.3155082372,0.7368587957

C,0,0.7983279105,1.5223538666,1.1335556993

C,0,-1.3533878461,0.7138264852,0.254724314

C,0,-1.4762296033,2.0694122866,-0.3723805035

C,0,-2.2244366078,-0.3390777407,-0.0318141852

C,0,-0.0602232182,-0.5460312771,1.9622279655

H,0,4.4919126528,-1.8027004,0.5706453704

H,0,5.1730926289,-1.229140955,-0.9691793213

H,0,5.2308361026,-0.1884744886,0.4465664096

H,0,4.0497122667,0.7063313039,-2.1762457859

H,0,2.446333838,1.2781598103,-1.6814720258

H,0,3.8845777952,1.705760805,-0.7393462909

H,0,2.2073771778,-1.7836821583,0.566739743

H,0,0.7407044887,0.2618194447,-1.2345278378

H,0,0.1099647161,-1.2767052668,-0.6107284765

H,0,0.9469567734,2.175847612,0.2737866807

H,0,0.2436070312,2.0511024018,1.9116668746

H,0,1.7675626672,1.1981042481,1.5169475917

H,0,0.9528961633,-0.756670065,2.31362182

H,0,-0.6139506554,0.0133745945,2.7193277954

H,0,-0.5929739276,-1.46149572,1.7096674214

H,0,-2.4924711253,2.1686851143,-0.7594124829

H,0,-1.3185846778,2.9078602176,0.3197281901

H,0,-0.7991735268,2.2314391798,-1.2318008532

O,0,-2.0693419516,-1.5651988174,0.1698724665

O,0,-3.4164334533,0.0936424632,-0.6010234716

C,0,-4.380686283,-0.9126869227,-0.8462576843

H,0,-5.2378440717,-0.4053471738,-1.2954342269

H,0,-4.0057158656,-1.6765265651,-1.5368300311

H,0,-4.6957160606,-1.4073838903,0.0800809651

Cleavage A Product

SM_Ylide_Cleavage_pdt/alanineprenylcleavageApdtm06631plusgstarstarpcm

Pdt Alanine ammonium dimethyl allyl ylide

um06/6-31+g**

E(UM06) = -636.530381159

Zero-point correction= 0.300024 (Hartree/Particle)

Thermal correction to Energy= 0.320057

Thermal correction to Enthalpy= 0.321002

Thermal correction to Gibbs Free Energy= 0.248323

Sum of electronic and zero-point Energies= -636.230357

Sum of electronic and thermal Energies= -636.210324

Sum of electronic and thermal Enthalpies= -636.209379

Sum of electronic and thermal Free Energies= -636.282058

E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	200.839	68.482	152.965

C	0.788524	-0.745480	-0.756150
C	2.061067	-1.027741	-0.293953
C	3.220938	-0.274400	-0.477519
C	3.260697	1.002263	-1.249789
C	4.520815	-0.716409	0.108370
N	-0.541974	0.880252	1.552228
C	0.598875	1.773010	1.514043
C	-1.662397	1.120586	0.804809
C	-1.808527	2.454129	0.146953
C	-2.589271	0.054839	0.543054
C	-0.450537	-0.133977	2.587437
H	4.424260	-1.647140	0.677644
H	5.277540	-0.871881	-0.675725
H	4.935304	0.052917	0.777692
H	4.012925	0.949022	-2.050284
H	2.301775	1.266106	-1.705532
H	3.565151	1.837621	-0.600697
H	2.177774	-1.941478	0.296263

H	0.566841	0.141446	-1.348632
H	-0.049132	-1.397265	-0.520387
H	0.665479	2.293628	0.556831
H	0.559573	2.515942	2.325595
H	1.513865	1.178831	1.633819
H	0.200106	-0.961819	2.271682
H	-0.017900	0.323471	3.487132
H	-1.432875	-0.536876	2.826393
H	-2.843246	2.615646	-0.158192
H	-1.187072	2.543777	-0.758142
H	-1.518009	3.267539	0.822033
O	-2.455259	-1.135945	0.845844
O	-3.702852	0.487903	-0.123075
C	-4.656144	-0.516411	-0.441686
H	-5.462678	-0.007872	-0.972162
H	-4.217089	-1.288009	-1.082612
H	-5.047672	-0.990955	0.464146

Cleavage A Transition State

SM_Ylide_Cleavage_ts/alanineprenylcleavageAtsm06631plusgstarstarpcm

alanine prenyl TSfreq

UM06/6-31+G**

E(UM06) = -636.521890517

Zero-point correction= 0.302763 (Hartree/Particle)

Thermal correction to Energy= 0.320520

Thermal correction to Enthalpy= 0.321464

Thermal correction to Gibbs Free Energy= 0.257307

Sum of electronic and ZPE= -636.219128

Sum of electronic and thermal Energies= -636.201371

Sum of electronic and thermal Enthalpies= -636.200426

Sum of electronic and thermal Free Energies= -636.264583

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	201.129	64.591	135.030

C,0,0.9741155078,-0.7469290698,-0.7177303483

C,0,2.2791967219,-1.0719821452,-0.2881627843

C,0,3.4267470259,-0.3456381407,-0.4895988684

C,0,3.4897464075,0.9178207493,-1.2836977437

C,0,4.7315548061,-0.8040648496,0.0740545055

N,0,-0.1601997931,0.3838372892,0.8048811019

C,0,0.7653604066,1.4890784249,1.0539571805

C,0,-1.4033411981,0.7279340447,0.2669416445

C,0,-1.5606560918,2.0786263997,-0.3593437142

C,0,-2.3530675192,-0.30896855,0.0256183634

C,0,-0.1267441106,-0.5435159444,1.9465420205

H,0,4.6310555966,-1.7263818215,0.655488188

H,0,5.466401604,-0.9784266506,-0.7256588603

H,0,5.1704411795,-0.0325589567,0.7240424625

H,0,4.2396520305,0.8299078873,-2.0826168561

H,0,2.5371287101,1.1961673451,-1.7433307199

H,0,3.8170868421,1.7556380703,-0.6501633722

H,0,2.3813130279,-1.9870170523,0.3016289396

H,0,0.8061886283,0.0614898526,-1.4276494708

H,0,0.1949577306,-1.5034626792,-0.6800478352

H,0,0.8714974869,2.1219856016,0.1718719193

H,0,0.4135937831,2.0984373106,1.8987530488

H,0,1.7452760435,1.070004167,1.3020379074

H,0,0.9091060579,-0.8540524775,2.1125633239

H,0,-0.4952970059,-0.0231538456,2.8419929801

H,0,-0.7479976215,-1.4127627629,1.7410343499

H,0,-2.5848670957,2.2048775709,-0.7114616087

H,0,-1.3456999928,2.8992733582,0.3371041829

H,0,-0.9007118779,2.2188685139,-1.2325997998

O,0,-2.2149093042,-1.5251625123,0.2234967309

O,0,-3.5326386272,0.1674687039,-0.4899637305

C,0,-4.523876527,-0.8109727057,-0.7637677308

H,0,-5.3771540481,-0.2674208928,-1.1734007666

H,0,-4.1670558613,-1.5457735419,-1.4932789167

H,0,-4.8244309226,-1.3387046904,0.1477472769

Polyrate Structures for C-N Bond Cleavage in Alanineprenyl Ammonium Salt

M062X/6-31+G/PCM**

Cleavage A Starting Material

SM_Ylide_Cleavage/alanineprenylcleavageAsmm062x631plusgstarstarpcm

SM Alanine ammonium dimethyl allyl ylide

m062x/6-31+g**

E(RM062X) = -636.698102848

Zero-point correction= 0.313086 (Hartree/Particle)

Thermal correction to Energy= 0.330026

Thermal correction to Enthalpy= 0.330970

Thermal correction to Gibbs Free Energy= 0.269062

Sum of electronic and ZPE= -636.385017

Sum of electronic and thermal Energies= -636.368077

Sum of electronic and thermal Enthalpies= -636.367132

Sum of electronic and thermal Free Energies= -636.429041

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	207.095	62.664	130.297

C,0,0.747521742,-0.4348997736,-0.4459999366

C,0,2.1199326319,-0.9234106488,-0.0966483499

C,0,3.2828206896,-0.3435762732,-0.4342826248

C,0,3.4163136471,0.94722555,-1.196758635

C,0,4.5944713013,-0.967449975,-0.0380639789

N,0,0.0299085751,0.3214789156,0.6782479157

C,0,0.8220653817,1.5364845074,1.0391098485

C,0,-1.3435003748,0.7119328852,0.2167639684

C,0,-1.4983005814,2.0767387566,-0.3950363102

C,0,-2.2229131309,-0.3369760684,-0.031796017

C,0,-0.0179574247,-0.5259582848,1.9174031375

H,0,4.4517330212,-1.8817954013,0.5416487751

H,0,5.1876569301,-1.2050992022,-0.928106092

H,0,5.1854025074,-0.262532433,0.5577313788

H,0,4.1112238766,0.8175383517,-2.0329587824

H,0,2.473267283,1.3262502146,-1.5919621845

H,0,3.8457686123,1.7176840449,-0.5448947182

H,0,2.161943132,-1.8576512481,0.4609885768

H,0,0.744437131,0.2548607312,-1.2916569835

H,0,0.0814803908,-1.2701038839,-0.6683566284

H,0,0.9447621429,2.1717750266,0.1644593621

H,0,0.2846452423,2.0734104665,1.8205153879

H,0,1.796992087,1.2133349181,1.4015924091

H,0,1.0034117477,-0.7049287849,2.2549961671

H,0,-0.5750447091,0.032887484,2.6687743025

H,0,-0.5281746495,-1.4547620406,1.6813486299

H,0,-2.5244690605,2.1648113033,-0.7507335082

H,0,-1.3261760684,2.9029704653,0.3037878579

H,0,-0.8442289952,2.2463914107,-1.2663325571

O,0,-2.0630867092,-1.5647256606,0.1830790882

O,0,-3.4283461653,0.0843015225,-0.5807295713

C,0,-4.3992360489,-0.931796737,-0.777148801

H,0,-5.2637169063,-0.4336675156,-1.2172750323

H,0,-4.0339266195,-1.7080365932,-1.4544166211

H,0,-4.6849106292,-1.3982400301,0.1699935271

Cleavage A Product

SM_Ylide_Cleavage_pdt/alanineprenylcleavageApdtm062x631plusgstarstarpcm

Pdt Alanine ammonium dimethyl allyl ylide

um062x/6-31+g**

E(UM062X) = -636.665411694

Zero-point correction= 0.304695 (Hartree/Particle)

Thermal correction to Energy= 0.324605

Thermal correction to Enthalpy= 0.325549

Thermal correction to Gibbs Free Energy= 0.253918

Sum of electronic and zero-point Energies= -636.360717

Sum of electronic and thermal Energies= -636.340807

Sum of electronic and thermal Enthalpies= -636.339863

Sum of electronic and thermal Free Energies= -636.411493

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	203.692	67.834	150.759
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.384626
C	1.107222	0.000000	2.232264
C	0.934996	0.016486	3.721017
C	2.523045	-0.015710	1.741828
N	0.112607	3.070949	-0.553587

C	-1.065275	3.425594	0.224545
C	1.353934	3.088724	0.204125
C	0.095620	2.788570	-1.885595
C	-1.115142	2.345301	-2.513740
O	-0.981794	2.208761	-3.869932
C	-2.141799	1.744720	-4.552442
C	1.389919	2.837266	-2.646576
O	-2.188741	2.081594	-1.956820
H	-0.118778	0.020803	4.010027
H	1.415856	-0.856815	4.181092
H	1.416698	0.900487	4.159786
H	3.049108	-0.902243	2.118576
H	2.601417	-0.012800	0.653619
H	3.070192	0.856177	2.124207
H	-0.974415	0.015563	1.874278
H	0.915284	-0.006662	-0.582869
H	-0.931819	0.046698	-0.551570
H	2.118310	2.485686	-0.284416
H	1.726456	4.112909	0.333497
H	1.161670	2.656567	1.191344
H	-1.453438	2.554104	0.764676
H	-0.771503	4.190256	0.949950

H -1.845893 3.818688 -0.421314

H 1.190855 2.939197 -3.711964

H 1.984064 1.923800 -2.507899

H 2.002139 3.683773 -2.323401

H -1.861570 1.682637 -5.603045

H -2.442180 0.761169 -4.183426

H -2.972998 2.442409 -4.424861

Cleavage A Transition State

SM_Ylide_Cleavage_ts/alanineprenylcleavageAtsm062x631plusgstarstarpcm

alanine prenyl TSfreq

UM062X/6-31+G**

E(UM062X) = -636.657111959

Zero-point correction= 0.307282 (Hartree/Particle)

Thermal correction to Energy= 0.324985

Thermal correction to Enthalpy= 0.325929

Thermal correction to Gibbs Free Energy= 0.261888

Sum of electronic and ZPE= -636.349830

Sum of electronic and thermal Energies= -636.332127

Sum of electronic and thermal Enthalpies= -636.331183

Sum of electronic and thermal Free Energies= -636.395224

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	203.931	64.003	134.785

C,0,0.9543247591,-0.725193676,-0.7985209082

C,0,2.2417647169,-1.0959935489,-0.345422005

C,0,3.405594593,-0.3775053144,-0.4666751392

C,0,3.5094320564,0.9350483123,-1.1875999658

C,0,4.6907614796,-0.8870857039,0.1179598918

N,0,-0.1580602163,0.433757153,0.7803333779

C,0,0.7804298115,1.5437451598,0.9652002873

C,0,-1.4034079941,0.7470558766,0.2618557626

C,0,-1.6188507022,2.1060497398,-0.3436082712

C,0,-2.3396172335,-0.3111101802,0.0367348371

C,0,-0.0625103828,-0.4985533267,1.9156894381

H,0,4.5534793543,-1.8390584129,0.6363257775

H,0,5.4476686979,-1.0242498686,-0.6649883528

H,0,5.1086786567,-0.1623884899,0.8287261739

H,0,4.2765045956,0.8779543127,-1.969760586

H,0,2.573224774,1.2479178361,-1.652230176

H,0,3.8278799665,1.7270720369,-0.4972140885

H,0,2.307866518,-2.0389565474,0.1981835458

H,0,0.8170632552,0.1167352926,-1.4696175614

H,0,0.1482507234,-1.4499394599,-0.7706636672

H,0,0.8451911036,2.1499311653,0.0632705044

H,0,0.4654438008,2.1714446755,1.8079100266

H,0,1.7638049719,1.1207344214,1.1792225879

H,0,0.9842624246,-0.7857430061,2.0307788319

H,0,-0.4012825715,0.0139703227,2.8243638774

H,0,-0.6724498222,-1.3761306693,1.7305719638

H,0,-2.6625258642,2.2142122198,-0.6313224424

H,0,-1.3731998442,2.9126211085,0.3542611557

H,0,-1.0105183232,2.25878654,-1.2472643383

O,0,-2.1667846388,-1.5223143436,0.2343204054

O,0,-3.5325876597,0.1348383669,-0.4661820275

C,0,-4.5016805297,-0.8739251451,-0.7306816716

H,0,-5.3687302715,-0.351349328,-1.1325365018

H,0,-4.1245289247,-1.5947165153,-1.4600216768

H,0,-4.7731192805,-1.4031950036,0.1858839344

Polyrate structures for Rearrangement of Glycineallylammonium salt M06/6-31+G/PCM(DMF)**

23 Starting Material

/g/home/biswas85/parentdmfm06/sm/g09.log

sm for 23 from opt of ts

M06/6-31+G**

E(RM06) = -518.694746359

Zero-point correction= 0.223875 (Hartree/Particle)

Thermal correction to Energy= 0.236917

Thermal correction to Enthalpy= 0.237861

Thermal correction to Gibbs Free Energy= 0.184158

Sum of electronic and ZPE= -518.470871

Sum of electronic and thermal Energies= -518.457829

Sum of electronic and thermal Enthalpies= -518.456885

Sum of electronic and thermal Free Energies= -518.510589

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.668	47.606	113.029

C,0,1.1333071034,-0.1218041045,2.2064736122

C,0,0.0000933671,0.0326690312,1.5220872205

C,0,-0.047768062,-0.0071633904,0.0354155882

N,0,-0.131398525,1.3843791958,-0.6153483973

C,0,1.0395596613,2.2399093241,-0.3350302844

C,0,2.3088823221,1.7771417278,-0.6612243047

O,0,3.2972129854,2.610343799,-0.164251276

C,0,4.628824054,2.248251984,-0.484027493

C,0,-1.3491782563,2.08477429,-0.1201183413

C,0,-0.2967356606,1.171366675,-2.090028071

O,0,2.6238708087,0.7659426221,-1.3222093789

H,0,0.8595729485,-0.4516936169,-0.3840109545

H,0,-0.9233939406,-0.5621344851,-0.3228546894

H,0,-0.9412142358,0.1729148895,2.0547282923

H,0,1.1511140466,-0.1082158632,3.2932473258

H,0,2.08387299,-0.274037335,1.6953626709

H,0,-1.2453061905,2.2752581971,0.9495823324

H,0,-2.224802973,1.4584105434,-0.309859651

H,0,-1.436868616,3.0343601354,-0.6523079255

H,0,-1.1789549197,0.5493744809,-2.2689146993

H,0,-0.4165303885,2.150844872,-2.556360578

H,0,0.6051424569,0.6844316774,-2.4629264389

H,0,4.8903416346,1.2661848778,-0.0731431755

H,0,5.2666192138,3.0118431856,-0.0333408849

H,0,4.7938065027,2.2276111707,-1.5673607619

H,0,0.8771776727,2.9881461163,0.4300172631

23 Product

/g/home/biswas85/parentdmfm06/p/g09.log

23 product

M06/6-31+G**

E(RM06) = -518.742159479

Zero-point correction= 0.223726 (Hartree/Particle)

Thermal correction to Energy= 0.236854

Thermal correction to Enthalpy= 0.237798

Thermal correction to Gibbs Free Energy= 0.184675

Sum of electronic and ZPE= -518.518434

Sum of electronic and thermal Energies= -518.505305

Sum of electronic and thermal Enthalpies= -518.504361

Sum of electronic and thermal Free Energies= -518.557485

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	148.628	47.081	111.808

C,0,0.248569026,0.1136980282,1.9585947295

C,0,0.5810526322,0.5139119792,0.5516588156

C,0,1.4829518537,-0.1172518565,-0.2011163179

N,0,-0.3509756572,2.094078552,3.3886020017

C,0,-0.916195782,2.8743330853,2.3009523105

C,0,0.6685419158,1.1187845757,3.0588438653

C,0,2.0285207211,1.6953505816,2.6839142054

O,0,2.2438670974,2.8169540825,2.2745605061

C,0,0.0017425704,2.9199325248,4.5294745891

O,0,2.9835199911,0.7685342633,2.8363855663

C,0,4.2950980678,1.1320048808,2.3921779129

H,0,2.031522176,-0.980237549,0.1776748281

H,0,1.7031314895,0.2007895908,-1.2172548827

H,0,0.0630272084,1.3794490129,0.1341369413

H,0,-0.8311290668,-0.0524686401,2.0776067804

H,0,0.7451077383,-0.8406958306,2.1717226977

H,0,0.3679930227,2.2869759032,5.34679906

H,0,-0.8904302817,3.4479418329,4.8860854284

H,0,0.7753996489,3.6750730397,4.3027152484

H,0,-1.7282384913,3.4898721524,2.7047200069

H,0,-0.1894061859,3.5442503473,1.8109286735

H,0,-1.3588969668,2.2186549574,1.5441576919

H,0,4.2774158229,1.3708354706,1.3243197181

H,0,4.9257013509,0.2625659108,2.5754419505

H,0,4.665355605,1.994536644,2.9526588523

H,0,0.8359234937,0.5278064607,3.9721138207

23 Transition State

/g/home/biswas85/parentdmfm06/ts/g09.log

glycine allyl TSfreq

M06/6-31+G**

E(RM06) = -518.672174429

Zero-point correction= 0.220896 (Hartree/Particle)

Thermal correction to Energy= 0.233692

Thermal correction to Enthalpy= 0.234636

Thermal correction to Gibbs Free Energy= 0.182582

Sum of electronic and ZPE= -518.451279

Sum of electronic and thermal Energies= -518.438483

Sum of electronic and thermal Enthalpies= -518.437539

Sum of electronic and thermal Free Energies= -518.489593

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 146.644 47.372 109.557

C,0,1.1208611714,-0.0012050587,2.1125085329

C,0,-0.1136273499,-0.2699158874,1.583957285

C,0,-0.3554501247,-0.0432927865,0.2254035237

N,0,-0.2145010566,2.0936215391,0.285248748

C,0,0.7811094194,2.4599781681,1.1635019884

C,0,2.1687937195,2.4265017896,0.8465109637

O,0,2.9104516828,2.9412969162,1.8715621034

C,0,4.3210402146,2.8385615063,1.7252096105

C,0,-1.5492321603,2.4601461294,0.7736762782

C,0,-0.0607426848,2.4096405313,-1.1429723496

O,0,2.7071323417,1.9863243866,-0.1723725164

H,0,0.4778537571,-0.0945258587,-0.4744652149

H,0,-1.3442334769,-0.1937334883,-0.2048344085

H,0,-0.9648707932,-0.3941218825,2.2551627538

H,0,1.2950406927,0.0104094622,3.1859679052

H,0,2.001846206,0.0291700209,1.4746665458

H,0,-1.6902623575,2.0613683712,1.782007574

H,0,-2.3089365272,2.0395412735,0.109954053

H,0,-1.6520779981,3.5531027327,0.7990406872

H,0,-0.8402921118,1.8839539589,-1.7024796709

H,0,-0.1727722291,3.4917198855,-1.2934349281

H,0,0.9239864679,2.0932252987,-1.4854614339

H,0,4.6303283239,1.7909198975,1.6392737064

H,0,4.7501679912,3.2779259748,2.6268805815

H,0,4.6701219697,3.3848655609,0.8431640978

H,0,0.4788829119,2.8076695588,2.1446875837

Polyrate Structures for Rearrangement of Glycineallylammonium Salt M062X/6-31+G/PCM(DMF)**

23 Starting Material

/g/home/biswas85/parentdmfm062x/sm/g09.log

sm for 23 from opt of ts

M062X/6-31+G**

E(RM062X) = -518.806416442

Zero-point correction= 0.227816 (Hartree/Particle)

Thermal correction to Energy= 0.240698

Thermal correction to Enthalpy= 0.241642

Thermal correction to Gibbs Free Energy= 0.188327

Sum of electronic and ZPE= -518.578601

Sum of electronic and thermal Energies= -518.565718

Sum of electronic and thermal Enthalpies= -518.564774

Sum of electronic and thermal Free Energies= -518.618090

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	151.040	46.846	112.212

C,0,1.1269700984,-0.0927661204,2.1998380003

C,0,-0.0129008803,0.0125338672,1.5175752732

C,0,-0.0474883799,-0.0139001263,0.0217496431

N,0,-0.130397807,1.3815076267,-0.6083299145

C,0,1.0402761819,2.2251171138,-0.3064318215

C,0,2.3061181091,1.7665970479,-0.6273198589

O,0,3.3019343985,2.6117448535,-0.1653461172

C,0,4.6299404757,2.2359724569,-0.5004037323

C,0,-1.3514869522,2.0757612902,-0.1048728894

C,0,-0.2819664972,1.1879828851,-2.0893205159

O,0,2.6202448181,0.7321195871,-1.2614781342

H,0,0.865124861,-0.4474256871,-0.3888032588

H,0,-0.9175385479,-0.5654183413,-0.345174927

H,0,-0.9598725925,0.1034004429,2.04542985

H,0,1.1427029289,-0.0861498449,3.2852017015

H,0,2.0793006265,-0.1905753062,1.6828505618

H,0,-1.2443265185,2.2440897797,0.9659222639

H,0,-2.2223069758,1.451383924,-0.3082977721

H,0,-1.4356258969,3.0309022681,-0.6227101229

H,0,-1.1599319664,0.5679842643,-2.2807280317

H,0,-0.398897612,2.1720384785,-2.5405527157

H,0,0.6238601914,0.7067678981,-2.45347295

H,0,4.8865725466,1.2615621939,-0.0761469306

H,0,5.2729916426,3.0053859662,-0.0726067502

H,0,4.7705520983,2.1963548627,-1.5840976165

H,0,0.8633976499,3.0361386192,0.3811237656

23 Product

/g/home/biswas85/parentdmfm062x/p/g09.log

23 product

M062X/6-31+G**

E(RM062X) = -518.851309696

Zero-point correction= 0.227403 (Hartree/Particle)

Thermal correction to Energy= 0.240398

Thermal correction to Enthalpy= 0.241342

Thermal correction to Gibbs Free Energy= 0.188355

Sum of electronic and ZPE= -518.623907

Sum of electronic and thermal Energies= -518.610912

Sum of electronic and thermal Enthalpies= -518.609967

Sum of electronic and thermal Free Energies= -518.662954

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	150.852	46.437	111.520

C,0,0.2296425962,0.1020687292,1.9668478427

C,0,0.5907750045,0.5243331986,0.565772539

C,0,1.5554705386,-0.0573767365,-0.1486883418

N,0,-0.3749900539,2.0828218482,3.4010598736

C,0,-0.8988159124,2.8625203808,2.285368259

C,0,0.6445902369,1.1004877434,3.0830345889

C,0,2.0107571184,1.6785164431,2.7104668553

O,0,2.2324637013,2.8175059376,2.3599329444

C,0,-0.0063993852,2.9257444314,4.5318839158

O,0,2.9572061051,0.735249234,2.7865595158

C,0,4.2628239655,1.1153961192,2.3335295749

H,0,2.1299130182,-0.8896672003,0.2528152446

H,0,1.7986930697,0.2782469706,-1.15204944

H,0,0.0470001625,1.3605850866,0.1298552668

H,0,-0.8501343369,-0.0556355602,2.0658316226

H,0,0.7230128483,-0.8510680536,2.1756191971

H,0,0.3357397267,2.2963081181,5.3590029712

H,0,-0.8882415714,3.4786140709,4.8673817744

H,0,0.786853976,3.6499042275,4.2911055698

H,0,-1.6780779637,3.5257379674,2.6704993707

H,0,-0.1361815918,3.4756046751,1.7835547196

H,0,-1.3684646599,2.202609606,1.5522652973

H,0,4.2183854803,1.4120907916,1.2834182847

H,0,4.8865462295,0.2326996962,2.4556848845

H,0,4.6455458043,1.9422884459,2.9340047246

H,0,0.8050548933,0.5100938292,3.9931179445

23 Transition State

/g/home/biswas85/parentdmfm062x/ts/g09.log

glycine allyl TSfreq

M062X/6-31+G**

E(RM062X) = -518.778941294

Zero-point correction= 0.225591 (Hartree/Particle)

Thermal correction to Energy= 0.237921

Thermal correction to Enthalpy= 0.238865

Thermal correction to Gibbs Free Energy= 0.187954

Sum of electronic and ZPE= -518.553350

Sum of electronic and thermal Energies= -518.541021

Sum of electronic and thermal Enthalpies= -518.540076

Sum of electronic and thermal Free Energies= -518.590988

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	149.297	45.928	107.152

C,0,1.0484463717,0.0846688271,2.1132030365

C,0,-0.1614101495,-0.2705747472,1.5631550875

C,0,-0.3432959294,0.0074895744,0.1999510948

N,0,-0.2054615318,2.0278568246,0.2999088228

C,0,0.7865572134,2.3597890321,1.2112700485

C,0,2.1728387466,2.3656063811,0.8720067357

O,0,2.9221821971,2.9288160568,1.8606939005

C,0,4.3350319755,2.8658711801,1.6763663018

C,0,-1.5377715433,2.4131060033,0.7965743704

C,0,-0.0334413512,2.4102371604,-1.1151786067

O,0,2.703664216,1.8865099367,-0.1322570412

H,0,0.5204906799,-0.0616541795,-0.4589825337

H,0,-1.3062367022,-0.1505056361,-0.2805148502

H,0,-1.0325621222,-0.3953812359,2.202425432

H,0,1.1947828465,0.1228165415,3.1892115398

H,0,1.9486300614,0.0549147309,1.5059560129

H,0,-1.6870080919,1.9720379731,1.7833393342

H,0,-2.2992672025,2.0402242754,0.1106424521

H,0,-1.6057018553,3.5032650623,0.8678237248

H,0,-0.8167434569,1.920250442,-1.6971625777

H,0,-0.1287442173,3.4961346546,-1.215509852

H,0,0.9454032707,2.0895274085,-1.4610260274

H,0,4.669196238,1.8280426814,1.6060366101

H,0,4.7687044122,3.3417313268,2.5544406899

H,0,4.6326640346,3.4009332869,0.7719360636

H,0,0.4796698898,2.8014344387,2.1480542311

Structures of Cation(SM), Most Stable [2,3]-TS and Diss-TS for p-Nitroglycine System

Guide to structures

SM=Cation

TS= Transition State

PS=6-31+G, SB=6-31G***

PCMDMSO=PCM model for DMSO

SM PBEPBED3 23PSPCMDMSO

home/biswas/quiver/sdPBE0

nitro SM

PBEPBE/6-31+g**

E(RPBE-PBE) = -876.713192634

Zero-point correction= 0.282979 (Hartree/Particle)

Thermal correction to Energy= 0.301037

Thermal correction to Enthalpy= 0.301981

Thermal correction to Gibbs Free Energy= 0.235281

Sum of electronic and ZPE= -876.430214

Sum of electronic and thermal Energies= -876.412156

Sum of electronic and thermal Enthalpies= -876.411212

Sum of electronic and thermal Free Energies= -876.477911

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	188.903	67.962	140.381

C,0,-0.8590705156,3.1526099243,0.2032767597

C,0,-0.1316177802,4.3131688126,-0.0347238254

C,0,0.0819384935,4.6918893688,-1.3536596229

C,0,-0.4097181784,3.9728257911,-2.4354832546

C,0,-1.1368622763,2.8167974541,-2.176829596

C,0,-1.3497709727,2.3881372412,-0.8618023592

C,0,-2.149980553,1.1426148447,-0.5823519393

N,0,-1.3216376681,-0.1442583944,-0.576678164

C,0,-0.1169112759,-0.0701096798,0.3111206801

C,0,-0.4110549377,0.224977751,1.7716764647

O,0,0.7257579444,0.2268179249,2.4442995608

C,0,0.6288948537,0.520542213,3.8525448645

C,0,-0.82037232,-0.4369329965,-1.9632052783

C,0,-2.2250528898,-1.2720382873,-0.1558158466

O,0,-1.5021932775,0.4419715693,2.2479862701

N,0,0.849895776,5.9203411358,-1.6165948485

O,0,1.2427467547,6.5633900877,-0.6583067375

O,0,1.0523986874,6.2277861649,-2.77869843

H,0,-1.0604935429,2.8533767007,1.227902539

H,0,0.2539746792,4.9153297675,0.7784823609

H,0,-0.2353915726,4.3160358157,-3.4475266165

H,0,-1.5519381423,2.2565053448,-3.0089477563

H,0,-2.6281419289,1.1964076172,0.3940641248

H,0,-2.9117436336,0.9834314775,-1.3475349495

H,0,-0.1248222263,0.3450884352,-2.2642963327

H,0,-1.6754993095,-0.473915156,-2.6376099509

H,0,-0.3145116123,-1.4015941527,-1.9491741075

H,0,-3.030216078,-1.3463819562,-0.8860189752

H,0,-2.6221879349,-1.0553675209,0.8329314099

H,0,-1.6407068126,-2.1917815968,-0.1460019948

H,0,0.5497037622,0.7048173684,-0.0753523541

H,0,0.4048695426,-1.027583566,0.2412637628

H,0,-0.0038691647,-0.2217940621,4.3396069645

H,0,1.6477517776,0.4695331342,4.2268883051

H,0,0.2123923327,1.5191664239,3.9900828731

TS PBEPBED3 23PSPCMDMSO

home/biswas/quiver/tdPBE0

Nitro TS

pbe1pbe/6-31+G**

E(RPBE1PBE) = -876.240582229

Zero-point correction= 0.275411 (Hartree/Particle)

Thermal correction to Energy= 0.292848

Thermal correction to Enthalpy= 0.293792

Thermal correction to Gibbs Free Energy= 0.229820

Sum of electronic and ZPE= -875.965171

Sum of electronic and thermal Energies= -875.947734

Sum of electronic and thermal Enthalpies= -875.946790

Sum of electronic and thermal Free Energies= -876.010762

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.765	65.523	134.640

SM B3LYPD3 23PSPCMDMSO

home/biswas/quiver/sdb3lypd3

nitro SM

b3lyp/6-31+g**

E(RB3LYP) = -877.753570008

Zero-point correction= 0.291679 (Hartree/Particle)

Thermal correction to Energy= 0.309143

Thermal correction to Enthalpy= 0.310087

Thermal correction to Gibbs Free Energy= 0.245142

Sum of electronic and ZPE= -877.461891

Sum of electronic and thermal Energies= -877.444427

Sum of electronic and thermal Enthalpies= -877.443483

Sum of electronic and thermal Free Energies= -877.508428

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	193.990	65.818	136.688

C,0,-0.1180088304,-0.0729390359,0.3384681583

C,0,-0.418607725,0.2153305541,1.8033264353

H,0,0.4122874144,-1.0241392088,0.2657229773

H,0,0.546912532,0.7064692228,-0.0378508654

O,0,-1.50998777,0.4742575818,2.2740488933

O,0,0.7197092151,0.1632405594,2.4850250651

C,0,0.6416874231,0.4526141877,3.9091800803

H,0,1.6629359175,0.3604968582,4.2719357118

H,0,0.2633316292,1.4653691991,4.0580091342

H,0,-0.0137189485,-0.271300075,4.3961497722

N,0,-1.3189215346,-0.1486847004,-0.5744896552

C,0,-0.7965337431,-0.4514944078,-1.9622302977

C,0,-2.2404123112,-1.2766273366,-0.1562757482

H,0,-1.6419217011,-0.4971386021,-2.647280103

H,0,-0.1034484889,0.3313742964,-2.263611616

H,0,-0.2844420845,-1.4125319978,-1.9392306714

H,0,-3.043547205,-1.3471866056,-0.8886622731

H,0,-1.6662257315,-2.2023992352,-0.1400052187

H,0,-2.6418912977,-1.057955763,0.8297965368

C,0,-2.1510801266,1.1568597791,-0.5968590271

H,0,-2.9110437078,0.9894373812,-1.3604594455

C,0,-1.3556063837,2.4057710146,-0.881278909

C,0,-0.8618328726,3.1789393766,0.1816862661

C,0,-0.1380105135,4.3431587973,-0.061882436

C,0,0.0746177634,4.7283383554,-1.3855224048

C,0,-0.4229367872,3.9964968656,-2.4639799757

C,0,-1.144431769,2.8351929869,-2.2008493334

H,0,-1.0528901258,2.879641172,1.2065835618

H,0,0.2475806649,4.9430667336,0.7521942125

N,0,0.8388878956,5.9569470026,-1.6537310162

H,0,-0.254636516,4.3331918327,-3.4786377582

H,0,-1.5533425089,2.2692785546,-3.0308397526

H,0,-2.6311796484,1.213800487,0.376761619

O,0,1.015827941,6.2871755148,-2.8292151528

O,0,1.267445935,6.5977556547,-0.690483764

TS B3LYPD3 23PSPCMDMSO

home/biswas/quiver/tdb3lypd3

Nitro TS

b3lyp/6-31+G**

E(RB3LYP) = -877.250602126

Zero-point correction= 0.273409 (Hartree/Particle)

Thermal correction to Energy= 0.290932

Thermal correction to Enthalpy= 0.291876

Thermal correction to Gibbs Free Energy= 0.227162

Sum of electronic and ZPE= -876.977193

Sum of electronic and thermal Energies= -876.959670

Sum of electronic and thermal Enthalpies= -876.958726

Sum of electronic and thermal Free Energies= -877.023440

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 182.563 65.840 136.202

C,0,-1.1335881879,-0.464536678,2.0781237071

C,0,-1.0358322865,-0.7287418892,3.4392357402

C,0,0.2054687744,-0.5929709788,4.0635252034

C,0,1.3464613083,-0.152429946,3.3661278462

C,0,1.2428568975,0.0853666346,2.009938159

C,0,0.0083400998,-0.0828211713,1.3286518778

C,0,-0.0715324581,-0.0844626839,-0.0989232353

N,0,-0.048758551,-2.0444256807,-0.5419381253

C,0,-0.876369562,-2.8018034052,0.2756203657

C,0,-0.4952569619,-3.3974341724,1.5126833191

O,0,-1.5935866839,-3.9954179483,2.0999825252

C,0,-1.3741998064,-4.5707609569,3.3965567838

C,0,1.4094949318,-2.3481737885,-0.5009964047

C,0,-0.5372621641,-1.9958300125,-1.949424647

O,0,0.618927479,-3.4486978142,2.0523264178

N,0,0.3198531553,-0.9163430957,5.4737512564

O,0,-0.6649582451,-1.3979136822,6.0562716803

O,0,1.4028791674,-0.7113001183,6.0438769737

H,0,-2.0957652813,-0.5466349695,1.5864937149

H,0,-1.8981040804,-1.0504270403,4.0090933182

H,0,2.287166305,-0.0348406694,3.8882991114

H,0,2.1210014473,0.3909466935,1.4494355338

H,0,-1.0415316862,0.1115124377,-0.5446283116

H,0,0.7740260332,0.2964616857,-0.6649397359

H,0,1.789472521,-2.1688654271,0.5002719031

H,0,1.9141838891,-1.7114399747,-1.2270574632

H,0,1.5559774066,-3.3999590729,-0.7583667337

H,0,0.0197802218,-1.2358737828,-2.4976839543

H,0,-0.3861143402,-2.9749523915,-2.4109173502

H,0,-1.5986351724,-1.7480227346,-1.9560303727

H,0,-1.9253409544,-2.7893232682,0.0160130221

H,0,-0.6047158516,-5.3469466966,3.3600306926

H,0,-1.0751715253,-3.8024776907,4.1166298341

H,0,-2.3308768386,-5.0044747112,3.6895563481

SM PBEPBED2 23PSPCMDMSO

home/biswas/quiver/sdPBEPBE-D2

nitro SM

PBEPBE/6-31+g**

E(RPBE-PBE) = -876.729137001

Zero-point correction= 0.282537 (Hartree/Particle)

Thermal correction to Energy= 0.300503

Thermal correction to Enthalpy= 0.301447

Thermal correction to Gibbs Free Energy= 0.235342

Sum of electronic and ZPE= -876.446600

Sum of electronic and thermal Energies= -876.428634

Sum of electronic and thermal Enthalpies= -876.427690

Sum of electronic and thermal Free Energies= -876.493795

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	188.568	67.912	139.129

C,0,-0.8523900911,3.1590112851,0.1946633117

C,0,-0.1165846268,4.3225783888,-0.0526951177

C,0,0.085726753,4.7134001882,-1.3839715711

C,0,-0.4327595661,3.9884356166,-2.4665249176

C,0,-1.1663995533,2.8276637989,-2.2001187536

C,0,-1.3690039497,2.394749901,-0.8730439869

C,0,-2.1654171072,1.148956395,-0.5856936558

N,0,-1.3207483165,-0.146408292,-0.5762580148

C,0,-0.1173220936,-0.0570735598,0.3313270412

C,0,-0.4245924748,0.2220616749,1.8004578474

O,0,0.7281945194,0.1875620699,2.4802583135

C,0,0.6274138705,0.4710744691,3.909237337

C,0,-0.8008745443,-0.4272001078,-1.9661961324

C,0,-2.2239429014,-1.2865171971,-0.1630162129

O,0,-1.5279330629,0.4585050112,2.2816366442

N,0,0.8612807495,5.9413826499,-1.6557432398

O,0,1.3061624368,6.5780849969,-0.6838066431

O,0,1.0302026721,6.2744452,-2.8425430176

H,0,-1.0404587729,2.8500139126,1.2267702039

H,0,0.2887682724,4.9233717658,0.7632296105

H,0,-0.2681081289,4.3352459255,-3.488039691

H,0,-1.5951859633,2.2618266162,-3.0316527108

H,0,-2.9321971034,0.9717085744,-1.3538234191

H,0,-2.6357966259,1.1956923434,0.4046965789

H,0,-0.1291616703,0.3875847863,-2.2664175051

H,0,-1.6613880444,-0.4940680736,-2.6454774032

H,0,-0.2569808034,-1.3810884153,-1.9445224113

H,0,0.4263558105,-1.0103243787,0.2444438364

H,0,0.5348415376,0.7416079195,-0.0557061483

H,0,-1.629871203,-2.2106400801,-0.1643796719

H,0,-3.0370546591,-1.3530759426,-0.8984218042

H,0,-2.6192810821,-1.0738148505,0.8374244027

H,0,-0.0278026787,-0.2721503196,4.387810085

H,0,1.6547979059,0.3948817677,4.2848964953

H,0,0.2240764953,1.4843229598,4.0567133205

TS PBEPBED2 23PSPCMDMSO

home/biswas/quiver/tdPBEPBE-D2

Nitro TS

PBEPBE/6-31+G**

E(RPBE-PBE) = -876.238062942

Zero-point correction= 0.265313 (Hartree/Particle)

Thermal correction to Energy= 0.283227

Thermal correction to Enthalpy= 0.284171

Thermal correction to Gibbs Free Energy= 0.218908

Sum of electronic and ZPE= -875.972750

Sum of electronic and thermal Energies= -875.954836

Sum of electronic and thermal Enthalpies= -875.953892

Sum of electronic and thermal Free Energies= -876.019155

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	177.727	67.734	137.358

C,0,-1.1359126153,-0.5047050043,2.1052737125

C,0,-1.0121064438,-0.7435137334,3.4747043215

C,0,0.24321462,-0.5699779984,4.0802911722

C,0,1.3705996775,-0.1231762886,3.3536242783

C,0,1.2413043189,0.0833625909,1.9856960343

C,0,-0.0060748972,-0.1165091278,1.3300343169

C,0,-0.1152433202,-0.1473498389,-0.1033122266

N,0,-0.0487165037,-2.0237558309,-0.5396866636

C,0,-0.890305979,-2.8187185474,0.2458940821

C,0,-0.5280718636,-3.406451144,1.4981450202

O,0,-1.6501187512,-4.0168617764,2.0597207732

C,0,-1.4308277129,-4.5975993779,3.3591455083

C,0,1.4127583869,-2.3157929089,-0.4622185827

C,0,-0.4920697179,-1.9868161553,-1.9653572936

O,0,0.5811932081,-3.4520721121,2.0674110982

N,0,0.3835395408,-0.856118919,5.5012030988

O,0,-0.5996210635,-1.3289362394,6.1177427538

O,0,1.4872624587,-0.6294328092,6.0488726703

H,0,-2.1087340799,-0.6152090016,1.6202930667

H,0,-1.8637726529,-1.0701711788,4.0744723195

H,0,2.3223346683,0.0234532594,3.8670943392

H,0,2.1101894707,0.3941989786,1.3973866732

H,0,-1.1077801932,0.0460813761,-0.5252531234

H,0,0.7162418864,0.2599021226,-0.6899105596

H,0,1.7521499488,-2.1647985919,0.5689628968

H,0,1.9317469148,-1.6408683082,-1.1573533306

H,0,1.573521952,-3.3656643137,-0.7523095574

H,0,0.0852133331,-1.2158514727,-2.495844938

H,0,-0.3134131275,-2.9756707172,-2.4151933263

H,0,-1.5635726775,-1.7452819184,-2.0018528694

H,0,-1.9410929795,-2.8013709396,-0.0437922447

H,0,-0.6417752882,-5.3677316332,3.3232495099

H,0,-1.1416790338,-3.8218415744,4.0904765801

H,0,-2.3920924844,-5.0487658662,3.6439794897

SM PBEPBED3 23PSPCMDMSO

/home/biswas/quiver/sdPBE0

nitro SM

pbe1pbe/6-31+g**

E(RPBE1PBE) = -876.748716869

Zero-point correction= 0.293658 (Hartree/Particle)

Thermal correction to Energy= 0.311083

Thermal correction to Enthalpy= 0.312027

Thermal correction to Gibbs Free Energy= 0.247054

Sum of electronic and ZPE= -876.455059

Sum of electronic and thermal Energies= -876.437634

Sum of electronic and thermal Enthalpies= -876.436690

Sum of electronic and thermal Free Energies= -876.501663

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	195.208	65.386	136.747

C,0,-0.8319701522,3.1910013439,0.1757162991

C,0,-0.111023036,4.3600629143,-0.0855747643

C,0,0.0738355209,4.745796058,-1.4198100623

C,0,-0.4503630261,4.0106377101,-2.4915399641

C,0,-1.1689831997,2.8445465854,-2.2114889524

C,0,-1.3510846391,2.4117610791,-0.8806463572

C,0,-2.1423070371,1.1636253232,-0.5775408744

N,0,-1.309478128,-0.1462216569,-0.5681783186

C,0,-0.1121587049,-0.0738492701,0.3538845328

C,0,-0.4282011141,0.1878520704,1.8246827939

O,0,0.7190590805,0.1359930211,2.5135360793

C,0,0.6146972082,0.4039670077,3.9445448302

C,0,-0.7787159924,-0.433537615,-1.9557028462

C,0,-2.233131933,-1.2774894709,-0.1640092314

O,0,-1.5333722725,0.4271650625,2.2999887047

N,0,0.8345211921,5.9792850931,-1.7063228673

O,0,1.2840026953,6.6247138672,-0.7423753062

O,0,0.9869698017,6.3072868183,-2.8966843691

H,0,-1.0048313742,2.8929436716,1.2136484553

H,0,0.2953495551,4.9687355795,0.7236990221

H,0,-0.3026946026,4.3535897823,-3.5167379568

H,0,-1.6021348609,2.2757663451,-3.0386860609

H,0,-2.9237166379,0.9901206468,-1.3310514228

H,0,-2.6039505145,1.2185578912,0.4163039712

H,0,-0.0829774231,0.3621281478,-2.2492941545

H,0,-1.6272608173,-0.4796103611,-2.6501547289

H,0,-0.257006247,-1.3989544841,-1.9372209349

H,0,0.4312253266,-1.026481144,0.2633111729

H,0,0.5516951836,0.723021297,-0.0152689639

H,0,-1.6536644672,-2.2096119414,-0.1486805867

H,0,-3.0362347605,-1.3444177055,-0.9088991985

H,0,-2.6449207332,-1.0616649803,0.8281001111

H,0,-0.0446062284,-0.339068552,4.4156240802

H,0,1.6392340077,0.3162594,4.3228849116

H,0,0.22076433,1.4178974659,4.1054559574

TS PBEPBED3 23PSPCMDMSO

/home/biswas/quiver/tdPBE0

Nitro TS

pbe1pbe/6-31+G**

C,0,-1.1308935553,-0.4577835354,2.0038841625

C,0,-1.0484594262,-0.7724927625,3.3531769892

C,0,0.1816518532,-0.6677685359,3.9931288393

C,0,1.3286566784,-0.1936649865,3.3311424877

C,0,1.2420421627,0.1055126175,1.9924786799

C,0,0.0172619176,-0.0360207244,1.2855204837

C,0,-0.0425541782,-0.0031775981,-0.1253084427

N,0,-0.0544884429,-2.0566827707,-0.5072767466

C,0,-0.8725113994,-2.7384873897,0.3475026108

C,0,-0.4769015961,-3.3534284878,1.5776029726

O,0,-1.5657627583,-3.9222684953,2.1724212281

C,0,-1.3302526738,-4.5119857608,3.4473026959

C,0,1.3910351189,-2.3366491617,-0.4601380747

C,0,-0.5575834544,-2.0179982706,-1.8926002842

O,0,0.6412388461,-3.4289328328,2.0858852755

N,0,0.2808522641,-1.0573440803,5.3766900675

O,0,-0.7020120801,-1.5649632736,5.9173832312

O,0,1.3497178726,-0.8806928029,5.9601425389

H,0,-2.0920848161,-0.500700959,1.5030574475

H,0,-1.9171995196,-1.1149883499,3.9030195758

H,0,2.2620010621,-0.0994312681,3.8730364453

H,0,2.1251071613,0.4428623831,1.4569723182

H,0,-1.007076286,0.1589616752,-0.597219954

H,0,0.8206164421,0.3426372049,-0.688535023

H,0,1.7750828704,-2.1157773546,0.5330462714

H,0,1.8852159858,-1.7192372211,-1.2101637537

H,0,1.5573162314,-3.3951592777,-0.6798199755

H,0,-0.0028682067,-1.2678675326,-2.4574703863

H,0,-0.4228789667,-3.0020935167,-2.351319048

H,0,-1.6171991526,-1.7612253625,-1.8880216883

H,0,-1.924192643,-2.7455932832,0.0936901902

H,0,-0.5665371044,-5.2919995081,3.3868462995

H,0,-1.0145139383,-3.7555757434,4.1730315468

H,0,-2.2835372688,-4.9439980349,3.7525000195

SM M11L 23PSPCMDMSO

home/biswas/quiver/sdM11L

nitro SM

M11L/6-31+g**

E(RM11L) = -877.417169463

Zero-point correction= 0.285056 (Hartree/Particle)

Thermal correction to Energy= 0.302715

Thermal correction to Enthalpy= 0.303660

Thermal correction to Gibbs Free Energy= 0.237757

Sum of electronic and ZPE= -877.132114

Sum of electronic and thermal Energies= -877.114454

Sum of electronic and thermal Enthalpies= -877.113510

Sum of electronic and thermal Free Energies= -877.179412

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	189.957	66.662	138.703

C,0,-0.8129223075,3.1693257364,0.1769591663

C,0,-0.1068895507,4.3277060579,-0.0858521189

C,0,0.0634317508,4.705445551,-1.4066632441

C,0,-0.4598426858,3.9810502825,-2.4643879249

C,0,-1.1618261172,2.8247820233,-2.1819794663

C,0,-1.3294267719,2.3979351254,-0.8645598266

C,0,-2.1091556409,1.1610553407,-0.5590450614

N,0,-1.2934533127,-0.1130965582,-0.5486234875

C,0,-0.1134104398,-0.0492139357,0.3428737239

C,0,-0.4199816823,0.2036409,1.7971488781

O,0,0.6992385636,0.1576976692,2.4658913108

C,0,0.5714018163,0.4086015294,3.8581050595

C,0,-0.7828716014,-0.3966900367,-1.9078711805

C,0,-2.1933086553,-1.2211084154,-0.1528709264

O,0,-1.500434179,0.4269558695,2.2603651669

N,0,0.805189292,5.9132782263,-1.6913653045

O,0,1.2620045462,6.5252655639,-0.7551077935

O,0,0.9279707487,6.2371465755,-2.8487661757

H,0,-0.984660429,2.8717815971,1.2171072046

H,0,0.3034903627,4.9403170925,0.7178383676

H,0,-0.3203508763,4.3268504283,-3.4895459961

H,0,-1.60217802,2.2529345751,-3.0048418851

H,0,-2.8915101381,0.9853890824,-1.3137224424

H,0,-2.5855169022,1.2224814187,0.4285769878

H,0,-0.0679698823,0.3811520872,-2.2038259797

H,0,-1.6284234048,-0.4261452284,-2.6063694602

H,0,-0.2803904007,-1.371693637,-1.8995502068

H,0,0.4300621466,-1.0013002311,0.2424591741

H,0,0.5615186118,0.7383322087,-0.0291178686

H,0,-1.6133841678,-2.1517363792,-0.1229249608

H,0,-2.9873344376,-1.3052631112,-0.9051714734

H,0,-2.6262777398,-1.007332284,0.8294472673

H,0,-0.0894838354,-0.337240691,4.3207771353

H,0,1.5844743009,0.3266095999,4.2622837467

H,0,0.1687870389,1.4168929672,4.0278425947

TS M11L 23PSPCMDMSO

home/biswas/quiver/tdM11L

Nitro TS

m11l/6-31+G**

E(RM11L) = -876.925441220

Zero-point correction= 0.267483 (Hartree/Particle)

Thermal correction to Energy= 0.284975

Thermal correction to Enthalpy= 0.285919

Thermal correction to Gibbs Free Energy= 0.222253

Sum of electronic and ZPE= -876.657958

Sum of electronic and thermal Energies= -876.640467

Sum of electronic and thermal Enthalpies= -876.639522

Sum of electronic and thermal Free Energies= -876.703189

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total 178.824 66.508 133.997

C,0,-1.133591421,-0.4701180496,2.075838161

C,0,-1.058749034,-0.730486061,3.4274120567

C,0,0.1734019915,-0.6273894072,4.0577379322

C,0,1.325847791,-0.2293607321,3.3770819473

C,0,1.2437006867,-0.000688729,2.0272795736

C,0,0.0198809727,-0.1330836217,1.3391521826

C,0,-0.0478458857,-0.1346635524,-0.0782786737

N,0,-0.0624420642,-2.0605726909,-0.5306737444

C,0,-0.8732623467,-2.8250263737,0.2589610156

C,0,-0.479998334,-3.3795472953,1.506976741

O,0,-1.5504000895,-3.942004352,2.1065154167

C,0,-1.2851744575,-4.4583537598,3.3789765533

C,0,1.3648936668,-2.3637644484,-0.5165958992

C,0,-0.5529196096,-1.9752678072,-1.9004295309

O,0,0.6203733489,-3.4178591369,2.0194315163

N,0,0.2620748774,-0.9392024401,5.4458699161

O,0,-0.7260207759,-1.3798895834,6.0010014221

O,0,1.3258058435,-0.7642743247,6.0070455388

H,0,-2.0998163794,-0.5251398017,1.5653549358

H,0,-1.941347822,-1.0196748278,4.001731532

H,0,2.2687500137,-0.1342065739,3.9174706081

H,0,2.1418910373,0.2823547317,1.4673781018

H,0,-1.018597144,0.0934211539,-0.5344486799

H,0,0.8157628399,0.2427393086,-0.6403228374

H,0,1.7841600029,-2.1873730107,0.4792980201

H,0,1.8605185184,-1.7257509304,-1.260742812

H,0,1.5129810166,-3.422517227,-0.7812734608

H,0,-0.0044435787,-1.189665606,-2.437945277

H,0,-0.4020219247,-2.9428942825,-2.4041431501

H,0,-1.624000495,-1.7346165123,-1.8948771626

H,0,-1.935454712,-2.7795751702,0.0200672728

H,0,-0.4928998716,-5.2235584279,3.3549258181

H,0,-0.9781395663,-3.6595849639,4.0793714857

H,0,-2.2246280954,-4.9064204946,3.7264424804

SM BP86D2 23PSPCMDMSO

home/biswas/quiver/sdBP86-D2

nitro SM

BP86/6-31+g**

E(RB-P86) = -877.776395535

Zero-point correction= 0.281581 (Hartree/Particle)

Thermal correction to Energy= 0.299543

Thermal correction to Enthalpy= 0.300487

Thermal correction to Gibbs Free Energy= 0.234399

Sum of electronic and ZPE= -877.494815

Sum of electronic and thermal Energies= -877.476853

Sum of electronic and thermal Enthalpies= -877.475909

Sum of electronic and thermal Free Energies= -877.541997

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	187.966	68.047	139.093

C,0,-0.8662221533,3.1425488558,0.2064174856

C,0,-0.1176515584,4.3017754147,-0.0324574321

C,0,0.094014491,4.6963029311,-1.3634423532

C,0,-0.4256643112,3.9799335809,-2.4538415993

C,0,-1.1717897561,2.8231502602,-2.1952567711

C,0,-1.3848086726,2.3884375985,-0.8691202775

C,0,-2.1839650933,1.1414049074,-0.5898418479

N,0,-1.3276343076,-0.1490190175,-0.5835366126

C,0,-0.1173854592,-0.0486799492,0.3178642509

C,0,-0.4225755767,0.2397228066,1.7879411519

O,0,0.7347252893,0.2235587173,2.4636580713

C,0,0.6348045995,0.5148034297,3.8963932414

C,0,-0.8128370451,-0.4253990646,-1.9793337527

C,0,-2.2194525509,-1.2992555384,-0.1636045985

O,0,-1.5278325699,0.4666121575,2.2725236949

N,0,0.883553895,5.9197091084,-1.6267198138

O,0,1.3331827661,6.5494015666,-0.6485284982

O,0,1.0607069924,6.259182219,-2.8136871816

H,0,-1.0622305133,2.8266631304,1.2353177267

H,0,0.2905901511,4.8954736726,0.7878295575

H,0,-0.2515628309,4.3294151142,-3.4734020482

H,0,-1.6006016965,2.261128005,-3.0299555875

H,0,-2.9453785164,0.961655758,-1.363699195

H,0,-2.6553710725,1.1812349299,0.4008990796

H,0,-0.1535093166,0.3998328669,-2.281847954

H,0,-1.6799981294,-0.501647508,-2.6505579958

H,0,-0.2573656435,-1.3736363221,-1.9579742111

H,0,0.4276592473,-1.00209305,0.2342272723

H,0,0.5275255859,0.7522311735,-0.0782349173

H,0,-1.614825171,-2.2175864187,-0.1726460301

H,0,-3.0378759948,-1.369186266,-0.8941701295

H,0,-2.6065396461,-1.0879192335,0.8412481174

H,0,-0.0078918418,-0.2377024648,4.3793229316

H,0,1.6661917618,0.4567831861,4.2668543455

H,0,0.2145806477,1.5229704426,4.0368748802

TS BP86D2 23PSPCMDMSO

home/biswas/quiver/tdBP86-D2

Nitro TS

BP86/6-31+G**

E(RB-P86) = -877.284243343

Zero-point correction= 0.264668 (Hartree/Particle)

Thermal correction to Energy= 0.282413

Thermal correction to Enthalpy= 0.283357

Thermal correction to Gibbs Free Energy= 0.219039

Sum of electronic and ZPE= -877.019575

Sum of electronic and thermal Energies= -877.001830

Sum of electronic and thermal Enthalpies= -877.000886

Sum of electronic and thermal Free Energies= -877.065204

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	177.217	67.720	135.368

C,0,-1.1577317107,-0.5327397048,2.0881633751

C,0,-1.0316177316,-0.8037153477,3.452955113

C,0,0.2268940859,-0.6437387287,4.0588641445

C,0,1.3520018164,-0.1676435115,3.3443755819

C,0,1.2202967459,0.0679207511,1.979345662

C,0,-0.0269187423,-0.1287777978,1.3214124078

C,0,-0.1328055442,-0.1618712114,-0.116456604

N,0,-0.0407947953,-2.0092823576,-0.547166375

C,0,-0.8762417994,-2.8235449777,0.2378397038

C,0,-0.5108872289,-3.3716058546,1.506428137

O,0,-1.6278769508,-3.9820116853,2.0881669268

C,0,-1.410185768,-4.4633944531,3.4320958849

C,0,1.4277227398,-2.2891425009,-0.467476274

C,0,-0.4797932791,-1.9898083634,-1.9789916349

O,0,0.5987634415,-3.3869273706,2.080569842

N,0,0.3729908021,-0.9820925799,5.4697946776

O,0,-0.5991625693,-1.5114620246,6.0639184338

O,0,1.4704918659,-0.7468979831,6.0325212314

H,0,-2.1289940536,-0.640341591,1.5987031251

H,0,-1.8811323103,-1.1490443743,4.0458867316

H,0,2.3040629389,-0.0308067697,3.8609451849

H,0,2.0878275263,0.3924067743,1.395329398

H,0,-1.1271683611,0.0322283297,-0.5369236255

H,0,0.6960318181,0.2592171189,-0.698782867

H,0,1.7610885123,-2.1262533088,0.5647628203

H,0,1.9381926922,-1.6117370662,-1.1681940643

H,0,1.5936352266,-3.3406085177,-0.7510265164

H,0,0.0912476602,-1.2133096357,-2.5103484496

H,0,-0.2846000298,-2.9809983829,-2.4182518177

H,0,-1.5552261708,-1.7620248929,-2.0176610513

H,0,-1.9275587384,-2.8109512951,-0.0523026317

H,0,-0.5861167558,-5.1974010011,3.4635334265

H,0,-1.1697272962,-3.6221875223,4.1088922777

H,0,-2.3584190365,-4.935467164,3.7306668257

SM BLYPD2 23PSPCMDMSO

home/biswas/quiver/sdBLYP-D2

nitro SM

BLYP/6-31+g**

E(RB-LYP) = -877.486350739

Zero-point correction= 0.281138 (Hartree/Particle)

Thermal correction to Energy= 0.299171

Thermal correction to Enthalpy= 0.300115

Thermal correction to Gibbs Free Energy= 0.233857

Sum of electronic and ZPE= -877.205212

Sum of electronic and thermal Energies= -877.187180

Sum of electronic and thermal Enthalpies= -877.186236

Sum of electronic and thermal Free Energies= -877.252494

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	187.732	68.331	139.452

C,0,-0.8791957499,3.162635898,0.1994712246

C,0,-0.1333374041,4.3268641171,-0.0373677602

C,0,0.0915084508,4.719008888,-1.3701171825

C,0,-0.4138382089,3.9910857587,-2.4635833426

C,0,-1.1575793852,2.8297179148,-2.2064724551

C,0,-1.3841383252,2.398892701,-0.8788354151

C,0,-2.1899115638,1.1494535394,-0.6024841976

N,0,-1.3329836114,-0.1587835629,-0.5851744699

C,0,-0.1160857591,-0.0645671371,0.3266552648

C,0,-0.4204152342,0.2310834573,1.8029153203

O,0,0.7422072078,0.2015085808,2.4802703162

C,0,0.6602673324,0.4976877917,3.9252990968

C,0,-0.811411459,-0.4476802102,-1.988701788

C,0,-2.2429383076,-1.309204564,-0.1625715041

O,0,-1.524485286,0.4728455257,2.2866846511

N,0,0.8799127945,5.951308663,-1.6321195309

O,0,1.3181017857,6.5959546164,-0.6486448939

O,0,1.0721503532,6.290441124,-2.8249397186

H,0,-1.0808729193,2.8514029458,1.2257919759

H,0,0.2608703996,4.9227001792,0.7849172257

H,0,-0.2327499602,4.3325859882,-3.4819518687

H,0,-1.5718184952,2.2626344343,-3.0418521874

H,0,-2.9410680078,0.9684884561,-1.3820677136

H,0,-2.6686498266,1.1912679191,0.3807537901

H,0,-0.1463616544,0.3698856801,-2.2897467456

H,0,-1.6765105655,-0.518709228,-2.6595027684

H,0,-0.2655025112,-1.3989153339,-1.9592523926

H,0,0.4177865583,-1.0215900632,0.2462729246

H,0,0.5328563576,0.7281092928,-0.070457001

H,0,-1.6442830615,-2.2291051926,-0.1632063263

H,0,-3.05408348,-1.3748635488,-0.8985506158

H,0,-2.6341407124,-1.089659408,0.8361563294

H,0,0.0127246403,-0.246015807,4.4115615964

H,0,1.6943519726,0.424694526,4.2810948979

H,0,0.2561896355,1.5106430584,4.065268264

TS BLYPD2 23PSPCMDMSO

home/biswas/quiver/tdBLYP-D2

Nitro TS

BLYP/6-31+G**

E(RB-LYP) = -876.994800740

Zero-point correction= 0.264159 (Hartree/Particle)

Thermal correction to Energy= 0.282111

Thermal correction to Enthalpy= 0.283056

Thermal correction to Gibbs Free Energy= 0.217527

Sum of electronic and ZPE= -876.730642

Sum of electronic and thermal Energies= -876.712689

Sum of electronic and thermal Enthalpies= -876.711745

Sum of electronic and thermal Free Energies= -876.777273

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	177.028	67.928	137.916

C,0,-1.1224342345,-0.5244481378,2.1795342936

C,0,-0.9866612516,-0.6786061626,3.5634909272

C,0,0.2761709761,-0.454693254,4.1504153066

C,0,1.4002829599,-0.0603298453,3.3819998769

C,0,1.2544394297,0.0664402948,2.0003571403

C,0,-0.0026769191,-0.1676332171,1.3736492092

C,0,-0.137333902,-0.2149822675,-0.0723449965

N,0,-0.0472539305,-2.0178676011,-0.5571626798

C,0,-0.9050138327,-2.8672635817,0.1906369268

C,0,-0.5578792873,-3.480137427,1.4310105716

O,0,-1.6947792336,-4.1179917789,1.971515632

C,0,-1.4880577226,-4.7461229384,3.2658975954

C,0,1.4285481188,-2.327953487,-0.4814804599

C,0,-0.4763258482,-1.9576741501,-2.0045660866

O,0,0.5486201404,-3.5389230655,2.0186832286

N,0,0.4269862468,-0.6294862189,5.5980042934

O,0,-0.5752883854,-0.99549913,6.275325347

O,0,1.5584304126,-0.4146598757,6.1184353226

H,0,-2.0938876695,-0.6788736798,1.7085421968

H,0,-1.8313838859,-0.972004237,4.1858708871

H,0,2.3566431847,0.1193247437,3.8714959695

H,0,2.1142673567,0.3443358625,1.3863034739

H,0,-1.1368565528,-0.0020520744,-0.4639364744

H,0,0.6738622935,0.2283865756,-0.658808425

H,0,1.7578917323,-2.2099716337,0.5544090632

H,0,1.9503328416,-1.6326738473,-1.1524997968

H,0,1.5751119618,-3.3683480052,-0.8048069762

H,0,0.1107836422,-1.179754266,-2.5117241162

H,0,-0.292698216,-2.9411929346,-2.459831146

H,0,-1.5459462155,-1.7128105737,-2.0434130273

H,0,-1.9508552447,-2.8202186309,-0.1061525526

H,0,-0.7117858809,-5.5269374357,3.2056374911

H,0,-1.1880443747,-3.9951163576,4.0163226023

H,0,-2.4589197095,-5.1882766622,3.5307783822

SM N12SX 23PSPCMDMSO

home/biswas/quiver/sdN12SX

nitro SM

N12SX/6-31+g**

E(RN12SX) = -877.275163094

Zero-point correction= 0.295536 (Hartree/Particle)

Thermal correction to Energy= 0.313023

Thermal correction to Enthalpy= 0.313967

Thermal correction to Gibbs Free Energy= 0.248478

Sum of electronic and ZPE= -876.979627

Sum of electronic and thermal Energies= -876.962140

Sum of electronic and thermal Enthalpies= -876.961196

Sum of electronic and thermal Free Energies= -877.026685

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	196.425	65.249	137.835

C,0,-0.8103543147,3.2190114726,0.1356536694

C,0,-0.1173483527,4.3859953069,-0.1448871547

C,0,0.0437346235,4.7559289683,-1.4723855859

C,0,-0.4750338182,4.0070077726,-2.5192861825

C,0,-1.1649343758,2.8430689674,-2.220268749

C,0,-1.3248049479,2.4275332342,-0.8953144855

C,0,-2.1021445049,1.1855837095,-0.5701501627

N,0,-1.283604435,-0.1056168132,-0.5413947564

C,0,-0.1081848865,-0.042699458,0.3806721508

C,0,-0.4275359919,0.1886067015,1.8415398465

O,0,0.6699399876,0.028609186,2.5514014903

C,0,0.5809121673,0.2486888878,3.9669943915

C,0,-0.7488322025,-0.4057438557,-1.9073785426

C,0,-2.206508829,-1.2191370555,-0.1449635198

O,0,-1.5084472809,0.4950411855,2.2926312479

N,0,0.7699927988,5.9810698685,-1.7774324439

O,0,1.2173392558,6.6341697757,-0.8439721443

O,0,0.8989895707,6.2975747582,-2.9526613523

H,0,-0.9648144397,2.9346966069,1.1671419126

H,0,0.2835450317,5.0020918229,0.6442262883

H,0,-0.3465173826,4.3350677943,-3.5385060623

H,0,-1.5921774049,2.2656241506,-3.027699243

H,0,-2.8775586222,1.0076503727,-1.3100856915

H,0,-2.5608936401,1.2629391082,0.4088477216

H,0,-0.0488916354,0.3689020806,-2.1996558947

H,0,-1.5799924676,-0.4478302228,-2.6033548047

H,0,-0.2448400803,-1.3660869441,-1.8793526369

H,0,0.4366545885,-0.9788058823,0.283698089

H,0,0.5512417023,0.7531955023,0.0398607675

H,0,-1.6380290887,-2.1426206237,-0.1086391279

H,0,-2.9883022965,-1.2957238059,-0.8929633856

H,0,-2.6338944416,-0.9964976254,0.8248515125

H,0,-0.1299126913,-0.447328712,4.4037074477

H,0,1.5776616051,0.0706349436,4.3515482568

H,0,0.2701127996,1.2712058218,4.1630901339

TS N12SX 23PSPCMDMSO

home/biswas/quiver/tdN12SX

Nitro TS

N12SX/6-31+G**

E(RN12SX) = -876.763523451

Zero-point correction= 0.277068 (Hartree/Particle)

Thermal correction to Energy= 0.294634

Thermal correction to Enthalpy= 0.295578

Thermal correction to Gibbs Free Energy= 0.230909

Sum of electronic and ZPE= -876.486455

Sum of electronic and thermal Energies= -876.468890

Sum of electronic and thermal Enthalpies= -876.467946

Sum of electronic and thermal Free Energies= -876.532614

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.885	65.464	136.106

C,0,-1.090237939,-0.4283357277,2.0573717124

C,0,-1.013114833,-0.6704636027,3.4166381426

C,0,0.2108003081,-0.525176859,4.0617199798

C,0,1.3628517131,-0.1121250013,3.3711104023

C,0,1.2826289706,0.11328428,2.0212669636

C,0,0.0569345628,-0.0405385435,1.3192890728

C,0,-0.0124475677,0.0062008834,-0.0830036006

N,0,-0.068183704,-2.1007861413,-0.5138910675

C,0,-0.8906656448,-2.7711518843,0.3309808525

C,0,-0.5033195407,-3.4473567999,1.5314146114

O,0,-1.5896984505,-4.0302861884,2.0995655016

C,0,-1.3725356996,-4.7433678338,3.3081104097

C,0,1.3725728373,-2.3895906657,-0.4829942527

C,0,-0.5828685335,-1.9948822772,-1.8884700017

O,0,0.6153150912,-3.5626070529,2.0258435106

N,0,0.2931593332,-0.7840367101,5.4657095914

O,0,-0.7183206131,-1.1612468838,6.0638803697

O,0,1.37746189,-0.6252360629,6.0331351277

H,0,-2.0467357707,-0.4931147292,1.5600209341

H,0,-1.883280386,-0.9697359238,3.9799084652

H,0,2.2910347021,0.0105287892,3.9066973674

H,0,2.1652506182,0.4191938796,1.4758712622

H,0,-0.9741910311,0.1580854591,-0.5512942505

H,0,0.8481411517,0.3348675391,-0.6501754331

H,0,1.7628207326,-2.2117338889,0.5106796126

H,0,1.8667625337,-1.7527396405,-1.2088423431

H,0,1.5325603918,-3.4354059416,-0.7435545493

H,0,-0.016004979,-1.2447445823,-2.4304608196

H,0,-0.4800506097,-2.9603872377,-2.3831933095

H,0,-1.6305495531,-1.7126088051,-1.8654168451

H,0,-1.9389529561,-2.7599417046,0.0825652224

H,0,-0.6505063076,-5.5447909631,3.1622657255

H,0,-1.0123220386,-4.0769690543,4.0905437207

H,0,-2.3360196785,-5.1568151249,3.5882969145

SM BP86 23PSPCMDMSO

home/biswas/quiver/sdBP86

nitro SM

BP86/6-31+g**

E(RB-P86) = -877.721657135

Zero-point correction= 0.281932 (Hartree/Particle)

Thermal correction to Energy= 0.300093

Thermal correction to Enthalpy= 0.301037

Thermal correction to Gibbs Free Energy= 0.234179

Sum of electronic and ZPE= -877.439725

Sum of electronic and thermal Energies= -877.421564

Sum of electronic and thermal Enthalpies= -877.420620

Sum of electronic and thermal Free Energies= -877.487478

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 188.311 68.296 140.714

C,0,-0.7714770209,3.2501031014,0.118352041

C,0,-0.0769449407,4.4268365436,-0.186997089

C,0,0.0406799514,4.8022872376,-1.5332977721

C,0,-0.5238628182,4.0498359824,-2.5741075703

C,0,-1.2142771631,2.8758861773,-2.2499271595

C,0,-1.3298968508,2.4522495014,-0.9063782928

C,0,-2.1069835016,1.2031483439,-0.5558110422

N,0,-1.2709516347,-0.1106756119,-0.5341921374

C,0,-0.087441391,-0.0434299054,0.412494866

C,0,-0.4355384015,0.152708938,1.8903664006

O,0,0.6739054638,-0.0548772079,2.6151360393

C,0,0.54538484,0.1495825801,4.0590875749

C,0,-0.7156628488,-0.3997086786,-1.915369089

C,0,-2.2044252792,-1.2447493568,-0.1461346512

O,0,-1.5317017602,0.4721266991,2.3421935588

N,0,0.7725969465,6.0428407426,-1.8663601179

O,0,1.2614461157,6.7041376708,-0.9288942328

O,0,0.8652366482,6.3632906337,-3.0679656154

H,0,-0.8935471323,2.9623965723,1.1668528582

H,0,0.3586129278,5.0488984957,0.5971494271

H,0,-0.4283228764,4.3849381237,-3.6085697272

H,0,-1.6775084056,2.2943262375,-3.0522431932

H,0,-2.9035857758,1.0093399975,-1.289392172

H,0,-2.545870846,1.2761077419,0.4482757554

H,0,-0.0079874274,0.3913446876,-2.1948936701

H,0,-1.5528563816,-0.4380832398,-2.6246689594

H,0,-0.2026757772,-1.3703056017,-1.8874886361

H,0,0.4812562925,-0.9780052398,0.2917735915

H,0,0.5597164292,0.7855980803,0.083640179

H,0,-1.621174211,-2.1743992418,-0.1054088968

H,0,-2.9853136401,-1.3216408664,-0.9140069851

H,0,-2.6463693517,-1.0200700467,0.831567819

H,0,-0.1967148521,-0.5510422401,4.4681286288

H,0,1.5443574319,-0.0566778936,4.4602605807

H,0,0.244463241,1.1874880423,4.262340689

TS BP86 23PSPCMDMSO

home/biswas/quiver/tdBP86

Nitro TS

BP86/6-31+G**

E(RB-P86) = -877.232413505

Zero-point correction= 0.264289 (Hartree/Particle)

Thermal correction to Energy= 0.282578

Thermal correction to Enthalpy= 0.283523

Thermal correction to Gibbs Free Energy= 0.216916

Sum of electronic and ZPE= -876.968124

Sum of electronic and thermal Energies= -876.949835

Sum of electronic and thermal Enthalpies= -876.948891

Sum of electronic and thermal Free Energies= -877.015497

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	177.321	68.330	140.185

C,0,-1.0743732676,-0.3905458835,2.233316883

C,0,-0.9607241437,-0.4528265133,3.6232585155

C,0,0.2963663965,-0.2250726977,4.2149709081

C,0,1.4406862562,0.0709942614,3.4371564099

C,0,1.317801662,0.1172674565,2.0527690286

C,0,0.0606386278,-0.1087587115,1.414419047

C,0,-0.0677199926,-0.1613100723,-0.0172240662

N,0,-0.0756116639,-2.0853775811,-0.5281706127

C,0,-0.9376319648,-2.8823689051,0.2262478266

C,0,-0.5814907183,-3.6208258078,1.4004819201

O,0,-1.7102934732,-4.290301518,1.8765054196

C,0,-1.4880344195,-5.1187974993,3.0383061603

C,0,1.3793638965,-2.4320209165,-0.4836211146

C,0,-0.5405483018,-1.9555115806,-1.9464166946

O,0,0.5280979339,-3.7463119726,1.9606404101

N,0,0.4170779514,-0.2792847111,5.6629025826

O,0,-0.6077921734,-0.5345157511,6.34502691

O,0,1.5452057824,-0.0716940637,6.1776855968

H,0,-2.0531128316,-0.5315213938,1.7661790001

H,0,-1.8254527884,-0.6661683004,4.2551428615

H,0,2.3969816224,0.2556733177,3.9304385589

H,0,2.1973460931,0.3424224418,1.4407560185

H,0,-1.0595346586,0.0500881033,-0.4301073592

H,0,0.7640713509,0.2230965391,-0.6182769855

H,0,1.7403941623,-2.3582611906,0.5480823043

H,0,1.9195282073,-1.7401476365,-1.143981753

H,0,1.505336064,-3.4671927372,-0.8384872791

H,0,0.0506345042,-1.1787811047,-2.4514622089

H,0,-0.4047435494,-2.9233792781,-2.4541917933

H,0,-1.6040596865,-1.6798134416,-1.9559474878

H,0,-1.9886904773,-2.8308582567,-0.0595204102

H,0,-0.7355901553,-5.8977004955,2.8312678855

H,0,-1.1544362162,-4.5140460154,3.8978232743

H,0,-2.4614010291,-5.5801630844,3.2556192437

SM wB97 23PSPCMDMSO

home/biswas/quiver/sdwB97

nitro SM

wB97/6-31+g**

E(RwB97) = -877.577445765

Zero-point correction= 0.295841 (Hartree/Particle)

Thermal correction to Energy= 0.313107

Thermal correction to Enthalpy= 0.314051

Thermal correction to Gibbs Free Energy= 0.249451

Sum of electronic and ZPE= -877.281605

Sum of electronic and thermal Energies= -877.264339

Sum of electronic and thermal Enthalpies= -877.263394

Sum of electronic and thermal Free Energies= -877.327995

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	196.478	64.911	135.963

C,0,-0.8430168603,3.1777115553,0.176566236

C,0,-0.1295778863,4.3460190993,-0.0737786431

C,0,0.0685470478,4.7233758016,-1.396561366

C,0,-0.4260940251,3.9916615113,-2.4698882541

C,0,-1.1373383014,2.8265686192,-2.2000387964

C,0,-1.3355366677,2.4020022966,-0.8803875001

C,0,-2.1325458274,1.1524331423,-0.5850756574

N,0,-1.3126165669,-0.1352537976,-0.5664162125

C,0,-0.1178378585,-0.0682327822,0.336134667

C,0,-0.415938228,0.2101849047,1.8019977221

O,0,0.7168144624,0.1501262989,2.4852591208

C,0,0.6193742404,0.4235034241,3.9036498114

C,0,-0.7988288264,-0.4365465567,-1.9450123235

C,0,-2.2260223793,-1.2547966166,-0.1512098954

O,0,-1.5051752442,0.4672759028,2.2757471596

N,0,0.8218070619,5.9619493128,-1.6726541836

O,0,1.2390634588,6.6031432564,-0.7207221527

O,0,0.9905770094,6.2818081181,-2.8391127683

H,0,-1.0309298768,2.8810775531,1.2078319557

H,0,0.2574604939,4.956133602,0.7367730123

H,0,-0.2653830847,4.3316539652,-3.4885202066

H,0,-1.5519014799,2.2560277085,-3.0294230422

H,0,-2.9027257795,0.9901575069,-1.3449331652

H,0,-2.6100288422,1.220530294,0.3938461514

H,0,-0.1008476909,0.3453897896,-2.2503668258

H,0,-1.6482910249,-0.4815128509,-2.6301340078

H,0,-0.2887858809,-1.4017989911,-1.9225242413

H,0,0.4094156834,-1.0244556784,0.2594221047

H,0,0.5537204667,0.7122462589,-0.0362812258

H,0,-1.6517904875,-2.1838923314,-0.1379514287

H,0,-3.0333658009,-1.3242391125,-0.8832686632

H,0,-2.626619436,-1.0364212976,0.8390531975

H,0,-0.0376768071,-0.3116728599,4.3750005026

H,0,1.6375044977,0.3359729486,4.2816935927

H,0,0.2311564401,1.4336770048,4.056798326

TS wB97 23PSPCMDMSO

home/biswas/quiver/tdwB97

Nitro TS

wB97/6-31+G**

E(RwB97) = -877.044276862

Zero-point correction= 0.277126 (Hartree/Particle)

Thermal correction to Energy= 0.294279

Thermal correction to Enthalpy= 0.295223

Thermal correction to Gibbs Free Energy= 0.232728

Sum of electronic and ZPE= -876.767151

Sum of electronic and thermal Energies= -876.749998

Sum of electronic and thermal Enthalpies= -876.749053

Sum of electronic and thermal Free Energies= -876.811549

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.663	65.336	131.533

C,0,-1.1206193559,-0.4516844103,1.9281171063

C,0,-1.0559175353,-0.807970015,3.2783993216

C,0,0.1630038729,-0.7423977174,3.9314121203

C,0,1.3307243506,-0.2490546624,3.3002756835

C,0,1.2629145014,0.1116234482,1.9812372506

C,0,0.0365959837,0.0135830307,1.2415085209

C,0,0.0029028034,0.1124213917,-0.1546288105

N,0,-0.063965513,-2.0893941421,-0.4956455383

C,0,-0.8754512931,-2.6688115913,0.4130411902

C,0,-0.4612232388,-3.3167901666,1.6425295376

O,0,-1.5459731579,-3.8605574336,2.2560950949

C,0,-1.3016281703,-4.4664793543,3.533337889

C,0,1.3846682397,-2.3564329341,-0.4584357692

C,0,-0.6021005865,-2.0453227101,-1.8688549548

O,0,0.6670792123,-3.4135873587,2.1186420625

N,0,0.2412321965,-1.1758219289,5.3146937291

O,0,-0.7356439748,-1.7290822285,5.8156338004

O,0,1.2862366166,-0.986066716,5.9303505159

H,0,-2.0866681823,-0.4328833466,1.4284620824

H,0,-1.9392652766,-1.1578285558,3.8067205694

H,0,2.2591662099,-0.183906492,3.8604028937

H,0,2.1546186318,0.4775560748,1.4727886914

H,0,-0.9546798785,0.2454625438,-0.6550822072

H,0,0.8854352692,0.4490510328,-0.6992376352

H,0,1.7901849168,-2.0630147389,0.5105329762

H,0,1.8560573852,-1.782003378,-1.2588359513

H,0,1.5603818217,-3.4274664984,-0.6132071975

H,0,-0.0404281487,-1.3117125905,-2.4516303892

H,0,-0.5048752619,-3.0375573042,-2.3254590321

H,0,-1.6556426766,-1.7578366304,-1.8374576205

H,0,-1.9316452633,-2.7053147654,0.1666193598

H,0,-0.5419652489,-5.2496604015,3.45050569

H,0,-0.9773404523,-3.7105225371,4.2590279857

H,0,-2.2578797971,-4.8945519138,3.8397300345

SM SOGGA11X 23PSPCMDMSO

home/biswas/quiver/sdSOGGA11X

nitro SM

SOGGA11X/6-31+g**

E(RSOGGA11X) = -877.445606973

Zero-point correction= 0.296738 (Hartree/Particle)

Thermal correction to Energy= 0.314140

Thermal correction to Enthalpy= 0.315085

Thermal correction to Gibbs Free Energy= 0.249792

Sum of electronic and ZPE= -877.148869

Sum of electronic and thermal Energies= -877.131467

Sum of electronic and thermal Enthalpies= -877.130522

Sum of electronic and thermal Free Energies= -877.195815

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	197.126	64.903	137.420

C,0,-0.8328844498,3.2255513992,0.1428416736

C,0,-0.1350408961,4.398970766,-0.130473649

C,0,0.0469389776,4.763078753,-1.4621457899

C,0,-0.4530994152,4.0084616245,-2.5208134955

C,0,-1.1483316074,2.8386503753,-2.2274439425

C,0,-1.3286798555,2.4275949514,-0.898591899

C,0,-2.1125049734,1.179330269,-0.5767074652

N,0,-1.2899957934,-0.1123681159,-0.5445157909

C,0,-0.103192327,-0.0467041046,0.3699903134

C,0,-0.4162227915,0.1974155392,1.837973211

O,0,0.6875088146,0.0224380919,2.5406244342

C,0,0.5921205996,0.257501506,3.9624237117

C,0,-0.7634798669,-0.4233415518,-1.9162966013

C,0,-2.2119138802,-1.2268112526,-0.1322773707

O,0,-1.4919416217,0.5235505992,2.2909058555

N,0,0.7800108449,5.9968525606,-1.7611007106

O,0,1.2057588153,6.6504958816,-0.8232093722

O,0,0.9274033757,6.3045928309,-2.9322834731

H,0,-1.0056275967,2.941758736,1.1768102416

H,0,0.2523020661,5.0217463434,0.6661949647

H,0,-0.3076577103,4.3346543241,-3.5430391404

H,0,-1.563515781,2.2556592078,-3.0435797698

H,0,-2.8862115756,0.9992672413,-1.3250954571

H,0,-2.5766867188,1.2576338656,0.4045001388

H,0,-0.0602284828,0.3517333739,-2.2173135488

H,0,-1.6044915316,-0.467648584,-2.6077735066

H,0,-0.2598128425,-1.3889827209,-1.8833492591

H,0,0.4370975442,-0.9908617307,0.2754664382

H,0,0.5579922274,0.7494315671,0.0187361153

H,0,-1.6391018634,-2.1532523687,-0.0958905034

H,0,-3.0027875634,-1.3060608243,-0.8773844555

H,0,-2.6316172741,-0.995521516,0.844061298

H,0,-0.1284690194,-0.4330522562,4.4017246861

H,0,1.5923205763,0.0709271089,4.3458694666

H,0,0.2906075959,1.2891151098,4.1466756517

TS SOGGA11X 23PSPCMDMSO

home/biswas/quiver/tdSOGGA11X

Nitro TS

SOGGA11X/6-31+G**

E(RSOGGA11X) = -876.925136810

Zero-point correction= 0.277851 (Hartree/Particle)

Thermal correction to Energy= 0.295356

Thermal correction to Enthalpy= 0.296300

Thermal correction to Gibbs Free Energy= 0.231690

Sum of electronic and ZPE= -876.647286

Sum of electronic and thermal Energies= -876.629781

Sum of electronic and thermal Enthalpies= -876.628837

Sum of electronic and thermal Free Energies= -876.693447

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	185.339	65.266	135.983

C,0,-1.1086661373,-0.4310663209,2.0158058156

C,0,-1.0368261654,-0.7214280226,3.374502355

C,0,0.1905149294,-0.6091529131,4.0254640115

C,0,1.3531581307,-0.1693693115,3.354538841

C,0,1.2771938334,0.1113853185,2.0110607077

C,0,0.0471662492,-0.0162642789,1.2941132073

C,0,-0.0084202707,0.0573594991,-0.1100376905

N,0,-0.0649992748,-2.1009296846,-0.5142390048

C,0,-0.8830150498,-2.74966388,0.3481085744

C,0,-0.4852276051,-3.4021337359,1.5710795427

O,0,-1.5733584492,-3.9750628781,2.1487227614

C,0,-1.3432580747,-4.6476663833,3.3875537965

C,0,1.3825891637,-2.3765758955,-0.4802812248

C,0,-0.5879632935,-2.0121644497,-1.8911069923

O,0,0.6358019066,-3.5001600852,2.0634363264

N,0,0.2691632134,-0.9282189437,5.4276653509

O,0,-0.7397674391,-1.3348029482,5.999342806

O,0,1.3469709172,-0.7871828757,6.0003010467

H,0,-2.0702208221,-0.4649439411,1.5151565967

H,0,-1.9148516706,-1.0354437738,3.9264609836

H,0,2.283957647,-0.0713231917,3.8997713225

H,0,2.1659781037,0.4396663562,1.4791354082

H,0,-0.9704482335,0.1985154735,-0.5918904793

H,0,0.8627637622,0.3903974819,-0.6680777884

H,0,1.7765344747,-2.1590601487,0.5095154043

H,0,1.8638846985,-1.7525281266,-1.2326920916

H,0,1.5530133774,-3.43313908,-0.710028065

H,0,-0.0236861608,-1.2589002403,-2.4408514177

H,0,-0.4806554327,-2.9858934682,-2.3798549891

H,0,-1.6415365522,-1.73356462,-1.8626056794

H,0,-1.9364844511,-2.7505821399,0.1016987278

H,0,-0.6198831267,-5.4566154183,3.2624521216

H,0,-0.9794849665,-3.9474842525,4.1441836731

H,0,-2.3116482308,-5.0500181212,3.6831850422

SM lc-B97D 23PSPCMDMSO

home/biswas/quiver/sdlc-B97D

nitro SM

lc-B97D/6-31+g**

E(RB97D) = -875.562615175

Zero-point correction= 0.298411 (Hartree/Particle)

Thermal correction to Energy= 0.314799

Thermal correction to Enthalpy= 0.315744

Thermal correction to Gibbs Free Energy= 0.253931

Sum of electronic and ZPE= -875.264204

Sum of electronic and thermal Energies= -875.247816

Sum of electronic and thermal Enthalpies= -875.246872

Sum of electronic and thermal Free Energies= -875.308685

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	197.540	63.055	130.096

C,0,-1.1414092629,2.9405569193,0.4610253841

C,0,-0.2997461338,4.0386117047,0.4292796117

C,0,0.2131722821,4.4278386494,-0.7956838331

C,0,-0.100303825,3.78262736,-1.9803983634

C,0,-0.9407763348,2.682891092,-1.926325059

C,0,-1.4388296006,2.2384500116,-0.7047220539

C,0,-2.2719309721,0.989906145,-0.6142579238

N,0,-1.4413408261,-0.2908054955,-0.6948294018

C,0,-0.1487447563,-0.2087615849,0.0593712794

C,0,-0.2956037216,0.3305665118,1.4650270162

O,0,0.7998849495,0.9654053213,1.8229327805

C,0,0.7602197246,1.6620718641,3.086449427

C,0,-1.0853804193,-0.589204121,-2.1198169559

C,0,-2.2894695529,-1.4208981298,-0.1885720355

O,0,-1.2894093971,0.2339306846,2.1456044156

N,0,1.1199808489,5.5850020527,-0.8432183294

O,0,1.3750685802,6.1572923097,0.1985102959

O,0,1.5748703971,5.9143020392,-1.9212581135

H,0,-1.5611659306,2.6139970348,1.4080173333

H,0,-0.0427572783,4.5815517064,1.3327225704

H,0,0.3039534366,4.1372183359,-2.9213345202

H,0,-1.2143112631,2.1753751286,-2.8465031902

H,0,-2.9952839265,0.9153660546,-1.4291311979

H,0,-2.7959538844,0.9519329193,0.3407080551

H,0,-0.4525599491,0.2103915364,-2.5042113109

H,0,-2.0125175548,-0.6620594503,-2.6914777498

H,0,-0.5455008919,-1.5381165471,-2.1400819852

H,0,0.2766428276,-1.2164181059,0.0894657266

H,0,0.5259476786,0.4435788826,-0.4975041632

H,0,-1.7223802591,-2.3459454179,-0.310254386

H,0,-3.1978785966,-1.4472304877,-0.7942184405

H,0,-2.5197454777,-1.2371741314,0.8598051899

H,0,0.493023793,0.9668913892,3.8856412407

H,0,1.7604990383,2.0692770543,3.2260353452

H,0,0.0163022579,2.4633877643,3.0187163418

TS lc-B97D 23PSPCMDMSO

home/biswas/quiver/tdlc-B97D

Nitro TS

lc-B97D/6-31+G**

E(RB97D) = -875.044816416

Zero-point correction= 0.278877 (Hartree/Particle)

Thermal correction to Energy= 0.295406

Thermal correction to Enthalpy= 0.296351

Thermal correction to Gibbs Free Energy= 0.235529

Sum of electronic and ZPE= -874.765940

Sum of electronic and thermal Energies= -874.749410

Sum of electronic and thermal Enthalpies= -874.748466

Sum of electronic and thermal Free Energies= -874.809287

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 185.370 63.923 128.010

C,0,-1.1951229566,-0.4615371422,1.9228299279

C,0,-1.0916686405,-0.8653441619,3.2471924555

C,0,0.1447121184,-0.8270368094,3.8575202777

C,0,1.2866694894,-0.3054799691,3.2138395069

C,0,1.1759343004,0.1152581251,1.9248612608

C,0,-0.0648360064,0.024646791,1.2242924285

C,0,-0.1179319386,0.0971180634,-0.1641735586

N,0,-0.0324587964,-2.0758198596,-0.4639780066

C,0,-0.835112507,-2.7044150219,0.4113779335

C,0,-0.438666797,-3.2609430242,1.6742413216

O,0,-1.5080030549,-3.8113527984,2.2942825397

C,0,-1.2890256795,-4.3196006578,3.6151523887

C,0,1.4263924715,-2.2431570428,-0.371587547

C,0,-0.5135093459,-2.0701030295,-1.8555209805

O,0,0.6700298426,-3.2731620868,2.1941205828

N,0,0.2818469187,-1.3592571275,5.192742379

O,0,-0.7111369816,-1.7931977796,5.7641203143

O,0,1.3905669085,-1.3788727692,5.7076824529

H,0,-2.1583768227,-0.4874770175,1.4236666043

H,0,-1.9479854242,-1.2744648964,3.7722057694

H,0,2.233077224,-0.2752634468,3.7412251267

H,0,2.0471873336,0.4895907993,1.3925101828

H,0,-1.0835694138,0.1606273568,-0.6584484829

H,0,0.7526477696,0.4222152747,-0.7293311268

H,0,1.7695310056,-1.9263113373,0.6119540035

H,0,1.8812103852,-1.6315641805,-1.1532351285

H,0,1.6713914749,-3.3011042318,-0.5170836182

H,0,0.0349763441,-1.3067526962,-2.4112429827

H,0,-0.3391181967,-3.0589725111,-2.2950345737

H,0,-1.5809401818,-1.8371718115,-1.8630281421

H,0,-1.8803815858,-2.783688181,0.1389045896

H,0,-0.4681169931,-5.0425217642,3.6138598497

H,0,-1.0565722679,-3.4994307805,4.3020192896

H,0,-2.2253509962,-4.7994692755,3.9036519621

SM B97D 23PSPCMDMSO

home/biswas/quiver/sdb97d

nitro SM

b97d/6-31+g**

E(RB97D) = -877.149087061

Zero-point correction= 0.284022 (Hartree/Particle)

Thermal correction to Energy= 0.301886

Thermal correction to Enthalpy= 0.302830

Thermal correction to Gibbs Free Energy= 0.236776

Sum of electronic and ZPE= -876.865065

Sum of electronic and thermal Energies= -876.847201

Sum of electronic and thermal Enthalpies= -876.846257

Sum of electronic and thermal Free Energies= -876.912311

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	189.436	67.619	139.022

C,0,-0.864714186,3.1624303108,0.1926384695

C,0,-0.124530357,4.3246715373,-0.0503354124

C,0,0.0881588837,4.716948747,-1.3809224696

C,0,-0.4264556241,3.9902289947,-2.465861264

C,0,-1.1642145697,2.8307529736,-2.2029798632

C,0,-1.3766422047,2.3990317227,-0.8773791823

C,0,-2.1772508839,1.1519874475,-0.5955701073

N,0,-1.3293397378,-0.1509556518,-0.5784688766

C,0,-0.1277218726,-0.0671029517,0.3418302387

C,0,-0.4346901123,0.2172117319,1.8159614358

O,0,0.7255195296,0.2020664927,2.4826906342

C,0,0.6564221644,0.4872686222,3.9194023018

C,0,-0.7956551872,-0.4329239222,-1.9709467399

C,0,-2.2429332456,-1.296723518,-0.1776281928

O,0,-1.5347752128,0.4375378144,2.3019253931

N,0,0.8719172529,5.9485715914,-1.6496149766

O,0,1.3122275848,6.583734619,-0.6796722134

O,0,1.0490373107,6.2817608902,-2.8310084908

H,0,-1.0570392367,2.8561660044,1.2196372901

H,0,0.2735479847,4.9179313078,0.7687263264

H,0,-0.2581588523,4.329252228,-3.4846316882

H,0,-1.5849593074,2.2667797246,-3.0340531934

H,0,-2.9319481005,0.9735929664,-1.3687748992

H,0,-2.6545256002,1.198368139,0.3856288771

H,0,-0.1208258805,0.3774381515,-2.2595010528

H,0,-1.6494961139,-0.4932511231,-2.6524590121

H,0,-0.2592073878,-1.3862646883,-1.9425696951

H,0,0.4042920239,-1.0219562563,0.2594778302

H,0,0.5273414919,0.7230942244,-0.0427615737

H,0,-1.6485939981,-2.2159506004,-0.1740644835

H,0,-3.041874725,-1.3580093153,-0.9230007283

H,0,-2.6491923994,-1.085759241,0.8135540403

H,0,0.0230271368,-0.2615885537,4.4098959799

H,0,1.6914005603,0.4214826164,4.265162274

H,0,0.2484188719,1.4939839638,4.0711860242

TS B97D 23PSPCMDMSO

home/biswas/quiver/tdb97d

Nitro TS

b97d/6-31+G**

E(RB97D) = -876.651803836

Zero-point correction= 0.266770 (Hartree/Particle)

Thermal correction to Energy= 0.284568

Thermal correction to Enthalpy= 0.285513

Thermal correction to Gibbs Free Energy= 0.220154

Sum of electronic and ZPE= -876.385034

Sum of electronic and thermal Energies= -876.367235

Sum of electronic and thermal Enthalpies= -876.366291

Sum of electronic and thermal Free Energies= -876.431650

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	178.569	67.265	137.560

C,0,-1.1134107729,-0.5097414179,2.1784996635

C,0,-0.980784999,-0.6560657082,3.5604533064

C,0,0.2773456008,-0.4332227718,4.147933189

C,0,1.4003264641,-0.0474766023,3.3804311738

C,0,1.2575675648,0.0748767427,2.0016912947

C,0,0.0044315798,-0.1577650226,1.3743904805

C,0,-0.1283071259,-0.2078410587,-0.0666834479

N,0,-0.048404333,-2.0208714295,-0.5429632166

C,0,-0.9014641325,-2.857936446,0.2090581267

C,0,-0.5522287072,-3.4949343072,1.435121091

O,0,-1.6884338465,-4.1162133433,1.9694338769

C,0,-1.490019582,-4.7847641977,3.232266062

C,0,1.4186174554,-2.3319468889,-0.4745315937

C,0,-0.4833815552,-1.9648273018,-1.9805170501

O,0,0.5528350545,-3.5843318883,2.0057825082

N,0,0.4248067299,-0.599309135,5.5954018782

O,0,-0.5689900127,-0.9546980227,6.2619675036

O,0,1.5428186702,-0.3851294348,6.1075607742

H,0,-2.0839562402,-0.661474995,1.7099838244

H,0,-1.8275910172,-0.9426626555,4.1790953937

H,0,2.3555075978,0.132176011,3.8671488475

H,0,2.1179492378,0.3491440529,1.3910298244

H,0,-1.1245692971,0.0065050992,-0.4591785543

H,0,0.6833038395,0.2294354245,-0.6528356852

H,0,1.7580218436,-2.2038248964,0.5539898475

H,0,1.9385552238,-1.6471165777,-1.1532713881

H,0,1.5627091519,-3.3730767102,-0.7872528143

H,0,0.1015159911,-1.1940030766,-2.495330489

H,0,-0.3074121394,-2.9482154555,-2.4328714634

H,0,-1.5494057964,-1.7163610773,-2.017181255

H,0,-1.9474700277,-2.8001542536,-0.0766449854

H,0,-0.7388612418,-5.5835030244,3.1431011024

H,0,-1.1661442185,-4.0700042669,4.0039402894

H,0,-2.4671879599,-5.2086803643,3.4925708847

SM wb97xd 23PSPCMDMSO

home/biswas/quiver/sdwb97xd

nitro SM

wb97xd/6-31+g**

E(RwB97XD) = -877.440850757

Zero-point correction= 0.295595 (Hartree/Particle)

Thermal correction to Energy= 0.312706

Thermal correction to Enthalpy= 0.313650

Thermal correction to Gibbs Free Energy= 0.249659

Sum of electronic and ZPE= -877.145255

Sum of electronic and thermal Energies= -877.128145

Sum of electronic and thermal Enthalpies= -877.127201

Sum of electronic and thermal Free Energies= -877.191192

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	196.226	64.731	134.680

C,0,-0.8544998713,3.1723852398,0.1822831534

C,0,-0.1353560787,4.3350201092,-0.062707682

C,0,0.0729761623,4.7142146303,-1.3824694936

C,0,-0.4204839053,3.9837473258,-2.4560734919

C,0,-1.1374555358,2.824143876,-2.19139801

C,0,-1.3442569488,2.3988313391,-0.8751942457

C,0,-2.1386306152,1.1518055765,-0.5857007908

N,0,-1.317249682,-0.1391396164,-0.5707132928

C,0,-0.1245253013,-0.0715605882,0.3358268575

C,0,-0.421941652,0.2097786847,1.7988686883

O,0,0.7132860625,0.1839434702,2.4719919205

C,0,0.6337428745,0.4614860485,3.8849052449

C,0,-0.7973454811,-0.4354766169,-1.9490266357

C,0,-2.2341011129,-1.2600117907,-0.1628353987

O,0,-1.5125779912,0.4391277334,2.275428127

N,0,0.8305694944,5.9425805451,-1.6532868475

O,0,1.2518873491,6.5807690775,-0.6985369781

O,0,1.0034076761,6.2656051053,-2.8204308978

H,0,-1.0456221275,2.8782168228,1.2090661885

H,0,0.2471983473,4.9366718621,0.7513614761

H,0,-0.2549977012,4.3187931652,-3.4717234159

H,0,-1.5459281618,2.2577821009,-3.0213709007

H,0,-2.907170852,0.9917535866,-1.3426416976

H,0,-2.6140729634,1.2142140959,0.3908420128

H,0,-0.0919887531,0.3392189483,-2.2440333527

H,0,-1.6395288137,-0.4674940562,-2.6386331851

H,0,-0.2976376629,-1.4027527534,-1.9307580639

H,0,0.4007468434,-1.0256255793,0.2610680871

H,0,0.5458773438,0.7046720662,-0.0383574269

H,0,-1.6625265006,-2.1870068215,-0.145793193

H,0,-3.0346368707,-1.3279676634,-0.8979086396

H,0,-2.6398399657,-1.0439235599,0.8222425023

H,0,-0.0064241929,-0.2751445187,4.3712612191

H,0,1.6552417607,0.3866483563,4.2483919987

H,0,0.2404308272,1.4665007988,4.0415691639

TS wb97xd 23PSPCMDMSO

home/biswas/quiver/tdwb97xd

Nitro TS

wb97xd/6-31+G**

E(RwB97XD) = -876.919262363

Zero-point correction= 0.276338 (Hartree/Particle)

Thermal correction to Energy= 0.293539

Thermal correction to Enthalpy= 0.294483

Thermal correction to Gibbs Free Energy= 0.231323

Sum of electronic and ZPE= -876.642925

Sum of electronic and thermal Energies= -876.625723

Sum of electronic and thermal Enthalpies= -876.624779

Sum of electronic and thermal Free Energies= -876.687939

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.199	65.314	132.932

C,0,-1.1334027661,-0.4499018599,1.9644646509

C,0,-1.0602841437,-0.7937460135,3.3100913411

C,0,0.1637417286,-0.7153719991,3.9574848141

C,0,1.3200689297,-0.2321407094,3.3116165567

C,0,1.2419249289,0.1105750386,1.9872599685

C,0,0.0173116049,-0.0015565487,1.2631085113

C,0,-0.0278340157,0.0801909408,-0.1368137546

N,0,-0.0519092919,-2.0836069385,-0.5032670591

C,0,-0.8602438922,-2.7113200081,0.3846806925

C,0,-0.4540582554,-3.3414220656,1.6132445948

O,0,-1.5394856432,-3.8880039397,2.222241565

C,0,-1.3097507335,-4.4797277631,3.5005015366

C,0,1.3985190067,-2.3389030192,-0.4638768346

C,0,-0.580463441,-2.0387261337,-1.8799377

O,0,0.6699835368,-3.4335274063,2.0989582958

N,0,0.2528425269,-1.1332940442,5.337116342

O,0,-0.7397875411,-1.6300258261,5.8708016916

O,0,1.3229035667,-0.9894163967,5.9274004893

H,0,-2.0949905889,-0.4656545191,1.4645084248

H,0,-1.9367787874,-1.1439516418,3.8407745979

H,0,2.2520684313,-0.1588266292,3.8572807218

H,0,2.1289322846,0.4629978734,1.4696155196

H,0,-0.9865325311,0.2153413381,-0.6263009759

H,0,0.8443486424,0.4205769912,-0.6877105686

H,0,1.7903379185,-2.0830671589,0.5175059359

H,0,1.8725083182,-1.73203584,-1.2341418776

H,0,1.5840350138,-3.3988736685,-0.6587946265

H,0,-0.0268927472,-1.2960316895,-2.453669255

H,0,-0.4672798557,-3.0242218306,-2.3408455586

H,0,-1.6352076225,-1.7663552713,-1.8556557551

H,0,-1.9131102521,-2.7340196889,0.1396716391

H,0,-0.5912998437,-5.2994289796,3.4287844468

H,0,-0.9436456964,-3.733051353,4.2104977665

H,0,-2.2782797892,-4.8574882396,3.8249928631

SM PBEPBE 23PSPCMDMSO

home/biswas/quiver/sdpbepbe

nitro SM

pbepbe/6-31+g**

E(RPBE-PBE) = -876.690079214

Zero-point correction= 0.282826 (Hartree/Particle)

Thermal correction to Energy= 0.300918

Thermal correction to Enthalpy= 0.301862

Thermal correction to Gibbs Free Energy= 0.235216

Sum of electronic and ZPE= -876.407253

Sum of electronic and thermal Energies= -876.389162

Sum of electronic and thermal Enthalpies= -876.388217

Sum of electronic and thermal Free Energies= -876.454864

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	188.829	68.068	140.269

C,0,-0.7781219121,3.2405591192,0.125826521

C,0,-0.0824945856,4.4161174879,-0.174252092

C,0,0.0439978424,4.7924848139,-1.5177824277

C,0,-0.5134020379,4.0413144092,-2.5611059011

C,0,-1.2056475787,2.8688558571,-2.242578873

C,0,-1.3303350202,2.444953855,-0.9017467357

C,0,-2.1080979212,1.1973154122,-0.5581400219

N,0,-1.2754096267,-0.1130306692,-0.5374631767

C,0,-0.092896453,-0.0461910005,0.4045849851

C,0,-0.4351145924,0.1586108549,1.8799045122

O,0,0.6783160733,-0.0330839826,2.5995633968

C,0,0.5539799936,0.1813094752,4.0376999909

C,0,-0.7242425688,-0.4014952133,-1.9161575447

C,0,-2.206190302,-1.2435500366,-0.1486708661

O,0,-1.5307102331,0.4713341645,2.3344196607

N,0,0.7768208632,6.0320011474,-1.8449561814

O,0,1.2546226653,6.6925038894,-0.9052010486

O,0,0.879361098,6.3496257445,-3.0434141235

H,0,-0.9061707529,2.9520633031,1.1730143151

H,0,0.348019811,5.0374151042,0.6127227633

H,0,-0.4110827795,4.3769963184,-3.5942872522

H,0,-1.6638937805,2.2881094614,-3.0477547544

H,0,-2.9021342198,1.0072063842,-1.2946678544

H,0,-2.5518520611,1.2691422069,0.4433087842

H,0,-0.0174078603,0.3887682915,-2.1978887485

H,0,-1.5619173146,-0.4401285255,-2.6241148739

H,0,-0.2113061733,-1.3715236205,-1.889959914

H,0,0.4719605408,-0.9831524401,0.2878857143

H,0,0.5580778927,0.7771892194,0.0707119847

H,0,-1.6246676564,-2.1737313419,-0.1104639072

H,0,-2.9892363294,-1.3196446434,-0.9136586062

H,0,-2.6456360412,-1.0205094175,0.8299947145

H,0,-0.1806521137,-0.5207738648,4.4566247292

H,0,1.5550217552,-0.0129118855,4.4384290871

H,0,0.2450073787,1.2176571217,4.2350867437

TS PBEPBE 23PSPCMDMSO

home/biswas/quiver/tdpbepbe

Nitro TS

pbepbe/6-31+G**

E(RPBE-PBE) = -876.201031323

Zero-point correction= 0.265314 (Hartree/Particle)

Thermal correction to Energy= 0.283474

Thermal correction to Enthalpy= 0.284418

Thermal correction to Gibbs Free Energy= 0.218256

Sum of electronic and ZPE= -875.935717

Sum of electronic and thermal Energies= -875.917557

Sum of electronic and thermal Enthalpies= -875.916613

Sum of electronic and thermal Free Energies= -875.982775

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	177.883	68.036	139.249

C,0,-1.0855909465,-0.4086811799,2.1965112877

C,0,-0.9856170248,-0.5088515176,3.5840538829

C,0,0.2656975747,-0.3075551585,4.1921633409

C,0,1.4171145178,0.0050142353,3.434429992

C,0,1.3083561551,0.0866946586,2.0520272279

C,0,0.0583026385,-0.117104585,1.3968937145

C,0,-0.0548126482,-0.1557359929,-0.0346835286

N,0,-0.0725840493,-2.0751410057,-0.5404984333

C,0,-0.9240954472,-2.8638497884,0.2302246731

C,0,-0.5549533429,-3.5709450028,1.4186197905

O,0,-1.675536475,-4.2234259335,1.9282136611

C,0,-1.4419574015,-4.9895483958,3.1249445662

C,0,1.3793714604,-2.4207512443,-0.5112507512

C,0,-0.5522008472,-1.9534604273,-1.9501439413

O,0,0.560202655,-3.6799427699,1.967546806

N,0,0.373244724,-0.4072324694,5.6378607406

O,0,-0.6547945942,-0.6864718297,6.2991707503

O,0,1.4934379658,-0.2137574207,6.1667783412

H,0,-2.0601874504,-0.5304061337,1.7167429591

H,0,-1.8570524224,-0.7345844555,4.2015715966

H,0,2.3691615157,0.1708210252,3.9414699919

H,0,2.1948268864,0.3202561383,1.454188625

H,0,-1.0399630351,0.0673304856,-0.4562790508

H,0,0.7864134761,0.223984889,-0.6243194046

H,0,1.7537129225,-2.3387095835,0.5143876332

H,0,1.9119274813,-1.7354383786,-1.1835835897

H,0,1.5008714561,-3.4584665409,-0.8583935583

H,0,0.029478406,-1.1767872598,-2.4651626845

H,0,-0.417418504,-2.921804174,-2.4559568418

H,0,-1.6165019724,-1.6832362325,-1.950501343

H,0,-1.9780312134,-2.8174887448,-0.0435865894

H,0,-0.6860854012,-5.7733823037,2.9548651553

H,0,-1.1064013133,-4.3401998698,3.9503639532

H,0,-2.4100467465,-5.4451580337,3.3729200272

SM MN12L 23PSPCMDMSO

home/biswas/quiver/sdMN12L

nitro SM

MN12L/6-31+g**

E(RMN12L) = -876.876416424

Zero-point correction= 0.293213 (Hartree/Particle)

Thermal correction to Energy= 0.310539

Thermal correction to Enthalpy= 0.311483

Thermal correction to Gibbs Free Energy= 0.246874

Sum of electronic and ZPE= -876.583203

Sum of electronic and thermal Energies= -876.565877

Sum of electronic and thermal Enthalpies= -876.564933

Sum of electronic and thermal Free Energies= -876.629543

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 194.866 65.237 135.983

C,0,-0.8821364529,3.1721887778,0.1907586281

C,0,-0.1510203461,4.3258622696,-0.0526498151

C,0,0.0746799616,4.6930058799,-1.374754442

C,0,-0.4128781382,3.9634773753,-2.4537478394

C,0,-1.1392489946,2.8113585312,-2.1901149927

C,0,-1.3646200287,2.3981174277,-0.8717289761

C,0,-2.1574538732,1.1551176197,-0.5878961691

N,0,-1.3157902437,-0.1211647229,-0.5604362185

C,0,-0.1131265658,-0.0362879608,0.323360652

C,0,-0.4031913934,0.2389645404,1.780955596

O,0,0.7234246278,0.1868568039,2.4552296375

C,0,0.630666878,0.4482160499,3.8618429151

C,0,-0.8083422689,-0.4187356143,-1.9379436702

C,0,-2.2110634956,-1.2478769978,-0.141698881

O,0,-1.4880989641,0.4854145187,2.2554488947

N,0,0.8398272104,5.8989038146,-1.6387373942

O,0,1.2937395395,6.518283365,-0.6801251614

O,0,0.9990106543,6.2399129923,-2.8077777657

H,0,-1.0981555062,2.8781834355,1.2158877452

H,0,0.2308855221,4.9366995714,0.7571956446

H,0,-0.2291522976,4.2980062662,-3.4682515412

H,0,-1.5483183537,2.2365220986,-3.0177231898

H,0,-2.9069045177,0.9728143058,-1.3646143177

H,0,-2.6549429526,1.2120414753,0.381552962

H,0,-0.1047955555,0.3588667328,-2.2397536648

H,0,-1.6593497627,-0.456075806,-2.620414675

H,0,-0.3038637181,-1.3859545878,-1.919312872

H,0,0.4268743446,-0.9846167915,0.2340030496

H,0,0.5467143424,0.7476894077,-0.0658760889

H,0,-1.6205556428,-2.1652392447,-0.1119916716

H,0,-3.0050952553,-1.3396214107,-0.8846879549

H,0,-2.6317686478,-1.0267042892,0.8379688362

H,0,-0.0163763588,-0.2933300287,4.3340131602

H,0,1.6468110273,0.3709406619,4.2399528001

H,0,0.2301812261,1.4499705332,4.0275797797

TS MN12L 23PSPCMDMSO

home/biswas/quiver/tdMN12L

Nitro TS

MN12L/6-31+G**

E(RMN12L) = -876.380845793

Zero-point correction= 0.275873 (Hartree/Particle)

Thermal correction to Energy= 0.292761

Thermal correction to Enthalpy= 0.293705

Thermal correction to Gibbs Free Energy= 0.231978

Sum of electronic and ZPE= -876.104973

Sum of electronic and thermal Energies= -876.088085

Sum of electronic and thermal Enthalpies= -876.087141

Sum of electronic and thermal Free Energies= -876.148868

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.710	64.982	129.915

C,0,-1.1665033538,-0.4768442902,2.0543049805

C,0,-1.067335681,-0.7900662943,3.3982257359

C,0,0.1836925447,-0.7120665996,4.0095421855

C,0,1.3275265417,-0.2663980844,3.3278943051

C,0,1.220197386,0.0242319093,1.9886927347

C,0,-0.0187181894,-0.1043164205,1.3108811791

C,0,-0.0977424401,-0.087286022,-0.1053353505

N,0,-0.046675802,-2.0595297412,-0.5321225224

C,0,-0.863984688,-2.8179559348,0.2738322484

C,0,-0.4845891587,-3.3297352387,1.5464056161

O,0,-1.5550184167,-3.9065555496,2.1539594885

C,0,-1.3228288741,-4.3712096277,3.4714377163

C,0,1.4063835124,-2.3072310737,-0.4753449386

C,0,-0.5201232874,-2.0008960462,-1.9269402959

O,0,0.6186548104,-3.3179746038,2.0899595954

N,0,0.3022012123,-1.0973579745,5.3814411652

O,0,-0.6861332011,-1.5762920883,5.9532236041

O,0,1.393466659,-0.9550819986,5.9460363061

H,0,-2.130232151,-0.5266830839,1.5537787424

H,0,-1.9320563333,-1.1075351412,3.9718630482

H,0,2.2717433721,-0.1896766866,3.8543882697

H,0,2.0980608698,0.3376575445,1.4272806474

H,0,-1.0716059325,0.0761839464,-0.5632255332

H,0,0.7552903231,0.2737565818,-0.6795569346

H,0,1.7884034591,-2.0669656958,0.5162731856

H,0,1.8840625723,-1.6859698134,-1.2355770046

H,0,1.5949519695,-3.3653578025,-0.6829813493

H,0,0.0190731572,-1.2122932748,-2.4561766943

H,0,-0.3349703375,-2.9653009579,-2.410162868

H,0,-1.5902233941,-1.7871590431,-1.9366068987

H,0,-1.9140860653,-2.819924659,0.0046756946

H,0,-0.534485589,-5.1292853378,3.4922523334

H,0,-1.0323876539,-3.5423370909,4.1303943163

H,0,-2.2657188409,-4.8005588069,3.8088762918

SM M11 23PSPCMDMSO

home/biswas/quiver/sdM11

nitro SM

M11/6-31+g**

E(RM11) = -877.257916048

Zero-point correction= 0.291517 (Hartree/Particle)

Thermal correction to Energy= 0.309007

Thermal correction to Enthalpy= 0.309951

Thermal correction to Gibbs Free Energy= 0.244755

Sum of electronic and ZPE= -876.966399

Sum of electronic and thermal Energies= -876.948909

Sum of electronic and thermal Enthalpies= -876.947965

Sum of electronic and thermal Free Energies= -877.013161

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	193.905	65.567	137.216

C,0,-0.8597174844,3.1570799009,0.1968525709

C,0,-0.1267074097,4.3125693584,-0.0473086855

C,0,0.0776764449,4.68640254,-1.3678062391

C,0,-0.4252491519,3.9726092979,-2.4463408731

C,0,-1.1549082864,2.8194674789,-2.1818875262

C,0,-1.3598456669,2.3945854134,-0.864802557

C,0,-2.1563415021,1.1444330973,-0.5776139639

N,0,-1.3153539453,-0.1316575257,-0.573390275

C,0,-0.1075357687,-0.0445045852,0.3072385986

C,0,-0.40303418,0.2316509427,1.7728443708

O,0,0.724152463,0.2079001505,2.4602181767

C,0,0.611674992,0.4816896865,3.8766760063

C,0,-0.8166765145,-0.4200645701,-1.9616831954

C,0,-2.20506196,-1.2679204758,-0.1477117393

O,0,-1.4965385563,0.461374933,2.2471736171

N,0,0.8548465682,5.9086671395,-1.6374235146

O,0,1.2897929643,6.5320980855,-0.682579406

O,0,1.0247039201,6.232898187,-2.8016281449

H,0,-1.0586247511,2.8553835264,1.2271233709

H,0,0.2731059022,4.9178472488,0.7639401066

H,0,-0.2535003019,4.3191245987,-3.4636006583

H,0,-1.5796295947,2.2548658224,-3.0135058072

H,0,-2.9232513081,0.9780724992,-1.3435890193

H,0,-2.6331034257,1.1989352749,0.4053565988

H,0,-0.1225101393,0.369222913,-2.2667159019

H,0,-1.6774060711,-0.4626669404,-2.6374035172

H,0,-0.3020068407,-1.3860975047,-1.9502458786

H,0,0.4355685982,-0.9946732759,0.2272614744

H,0,0.5463466517,0.7505009258,-0.074758255

H,0,-1.6089993673,-2.1864626416,-0.1328993079

H,0,-3.0134705601,-1.3566436624,-0.8806612556

H,0,-2.6083839152,-1.049576647,0.8439926903

H,0,-0.0308883744,-0.2733052579,4.342529445

H,0,1.6298350548,0.4263857416,4.2666389301

H,0,0.1876075164,1.4816153243,4.0212227645

TS M11 23PSPCMDMSO

home/biswas/quiver/tdM11

Nitro TS

M11/6-31+G**

E(RM11) = -876.740360678

Zero-point correction= 0.273446 (Hartree/Particle)

Thermal correction to Energy= 0.290667

Thermal correction to Enthalpy= 0.291611

Thermal correction to Gibbs Free Energy= 0.229147

Sum of electronic and ZPE= -876.466915

Sum of electronic and thermal Energies= -876.449694

Sum of electronic and thermal Enthalpies= -876.448750

Sum of electronic and thermal Free Energies= -876.511214

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.396	65.765	131.467

C,0,-1.1384489049,-0.5078815365,1.9224563671

C,0,-1.061195569,-0.8690389485,3.2677588368

C,0,0.1607720626,-0.782617463,3.912387668

C,0,1.3176664549,-0.271489505,3.2809779783

C,0,1.2350362751,0.1023072508,1.9682650959

C,0,0.0065804817,-0.0082382748,1.2359538199

C,0,-0.0386538142,0.119156303,-0.1524343772

N,0,-0.0581340011,-2.1046924156,-0.4978663639

C,0,-0.8764723145,-2.6764325464,0.3969433656

C,0,-0.4684239065,-3.290505319,1.6456808855

O,0,-1.5469213989,-3.8307133241,2.2656948458

C,0,-1.2935902371,-4.4202490862,3.54731351

C,0,1.3976106549,-2.3187821763,-0.4170078901

C,0,-0.5668238178,-2.0450998553,-1.881948277

O,0,0.654737651,-3.3621391948,2.1325127948

N,0,0.2517342229,-1.2082346733,5.2913041254

O,0,-0.7431497865,-1.6900565375,5.8299662249

O,0,1.3255287877,-1.081246662,5.8741677008

H,0,-2.107740052,-0.5038517176,1.4232575668

H,0,-1.9344733754,-1.2422803059,3.8025943481

H,0,2.247991886,-0.1971648377,3.8407902949

H,0,2.1173540815,0.4909991384,1.455513013

H,0,-1.0039160121,0.218129159,-0.6509402515

H,0,0.8379364043,0.4691446912,-0.7024914436

H,0,1.7642108812,-1.9927590864,0.5601250468

H,0,1.8679473043,-1.7408516593,-1.2187751058

H,0,1.6141204976,-3.3884849458,-0.5439981135

H,0,-0.000111297,-1.2918387353,-2.438596004

H,0,-0.4430000753,-3.0302112046,-2.3525451083

H,0,-1.6271859413,-1.772808307,-1.8667931223

H,0,-1.9306743671,-2.7355663345,0.1367090798

H,0,-0.5467613306,-5.2187699688,3.4596360244

H,0,-0.9335529878,-3.6564285715,4.250561975

H,0,-2.2517094566,-4.8253183498,3.8844144897

SM N12 23PSPCMDMSO

home/biswas/quiver/sdN12 nitro SM

N12/6-31+g**

E(RN12) = -877.560264044

Zero-point correction= 0.290287 (Hartree/Particle)

Thermal correction to Energy= 0.307979

Thermal correction to Enthalpy= 0.308923

Thermal correction to Gibbs Free Energy= 0.243318

Sum of electronic and ZPE= -877.269977

Sum of electronic and thermal Energies= -877.252285

Sum of electronic and thermal Enthalpies= -877.251341

Sum of electronic and thermal Free Energies= -877.316946

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	193.260	66.474	138.078

C,0,-0.7960594967,3.2309686411,0.1293739597

C,0,-0.1118813237,4.4012360495,-0.1578197822

C,0,0.0424727571,4.7687008837,-1.4881446774

C,0,-0.4773163625,4.0110678412,-2.5299937003

C,0,-1.1605919529,2.8452299169,-2.2243058209

C,0,-1.3119444446,2.4312029307,-0.8962111108

C,0,-2.0882884542,1.1947312116,-0.5604130567

N,0,-1.2786276391,-0.107319896,-0.5384794754

C,0,-0.1056388054,-0.0492408057,0.3878203897

C,0,-0.4341617129,0.1696297283,1.8499250496

O,0,0.6622876042,0.0044316718,2.5612998534

C,0,0.568416349,0.2194728522,3.9769896505

C,0,-0.7442861928,-0.4052959127,-1.903540262

C,0,-2.2088904626,-1.213918388,-0.1432994772

O,0,-1.5184497195,0.4709164999,2.2983783869

N,0,0.7577046316,5.9950544157,-1.7999026451

O,0,1.1963674281,6.6649613791,-0.8655075148

O,0,0.8914677626,6.3036670636,-2.9836278896

H,0,-0.9437894923,2.9514118101,1.1607925332

H,0,0.2863291676,5.0227456938,0.6259609914

H,0,-0.3553129165,4.3367031391,-3.5489797727

H,0,-1.5885556339,2.2658778315,-3.0272834538

H,0,-2.8735440137,1.0177407581,-1.287456221

H,0,-2.5289294838,1.2708192011,0.4256634997

H,0,-0.0426188044,0.3669801947,-2.190410583

H,0,-1.574251497,-0.4424328396,-2.5980473738

H,0,-0.2448774506,-1.3659195636,-1.8762987747

H,0,0.4398102671,-0.9819763549,0.2822620954

H,0,0.5495733077,0.7497364964,0.0518337822

H,0,-1.6471394475,-2.1393517136,-0.1078487682

H,0,-2.990877692,-1.2827226699,-0.8888823778

H,0,-2.6300360486,-0.9869344208,0.8262321802

H,0,-0.1141034824,-0.5020194895,4.4141867356

H,0,1.5712873805,0.0774572126,4.3565678667

H,0,0.2210218742,1.2281956319,4.1746787631

TS N12 23PSPCMDMSO

home/biswas/quiver/tdN12

Nitro TS

N12/6-31+G**

E(RN12) = -877.063939794

Zero-point correction= 0.271978 (Hartree/Particle)

Thermal correction to Energy= 0.289830

Thermal correction to Enthalpy= 0.290774

Thermal correction to Gibbs Free Energy= 0.225168

Sum of electronic and ZPE= -876.791962

Sum of electronic and thermal Energies= -876.774110

Sum of electronic and thermal Enthalpies= -876.773166

Sum of electronic and thermal Free Energies= -876.838771

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	181.871	66.669	138.079

C,0,-1.0662536845,-0.3928300737,2.2028606293

C,0,-0.9691301649,-0.4688502121,3.5785459789

C,0,0.2698466214,-0.2575622384,4.1822566963

C,0,1.4129154743,0.0358480221,3.4255908929

C,0,1.3075870584,0.0978519995,2.0555267785

C,0,0.0678193651,-0.1109519905,1.40626358

C,0,-0.0454192147,-0.1523392393,-0.0081609161

N,0,-0.0767259493,-2.0917309749,-0.5095143151

C,0,-0.9221160568,-2.8555646134,0.2592154425

C,0,-0.5564722942,-3.596969401,1.4147715266

O,0,-1.6545095547,-4.2361667514,1.9151151878

C,0,-1.4428126686,-5.0637535608,3.0457089853

C,0,1.357497686,-2.4318764729,-0.4798375388

C,0,-0.5562083483,-1.9554148041,-1.8987435769

O,0,0.5510123123,-3.7335239286,1.9365645758

N,0,0.3729233209,-0.329067249,5.6059144719

O,0,-0.6474039976,-0.574352195,6.2688029087

O,0,1.4827919926,-0.1460342229,6.1307211225

H,0,-2.0271427773,-0.5216962574,1.7306323983

H,0,-1.8304480388,-0.6808894386,4.1894138236

H,0,2.3514329735,0.2061173051,3.9253792995

H,0,2.1835425625,0.3193648329,1.4644653379

H,0,-1.018111552,0.0504853528,-0.4297627613

H,0,0.7860885123,0.205562591,-0.5976398698

H,0,1.72840689,-2.3583477623,0.5319668291

H,0,1.8853684902,-1.7523564758,-1.1375086094

H,0,1.4824292936,-3.4536050633,-0.8283160809

H,0,0.0172397691,-1.1881442788,-2.405767677

H,0,-0.4309963092,-2.906174337,-2.4099093145

H,0,-1.6054157244,-1.6846059575,-1.8943074169

H,0,-1.9630959048,-2.8036546124,-0.0057160942

H,0,-0.7655297513,-5.8820012671,2.809617389

H,0,-1.0327427549,-4.4947055428,3.8767932351

H,0,-2.4180785761,-5.4560761822,3.3106460816

SM B3LYP 23PSPCMDMSO

home/biswas/quiver/sdb3lyp

nitro SM

b3lyp/6-31+g**

E(RB3LYP) = -877.714104651

Zero-point correction= 0.291006 (Hartree/Particle)

Thermal correction to Energy= 0.308685

Thermal correction to Enthalpy= 0.309629

Thermal correction to Gibbs Free Energy= 0.243990

Sum of electronic and ZPE= -877.423099

Sum of electronic and thermal Energies= -877.405420

Sum of electronic and thermal Enthalpies= -877.404476

Sum of electronic and thermal Free Energies= -877.470115

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	193.702	66.229	138.149

C,0,-0.8143055742,3.2544949934,0.125372289

C,0,-0.1246706488,4.4298649302,-0.1622917959

C,0,0.0396491164,4.79352824,-1.498249117

C,0,-0.4745729849,4.0298720362,-2.5459926924

C,0,-1.1616227547,2.8583012974,-2.2390582243

C,0,-1.3225937114,2.4468818168,-0.9055037089

C,0,-2.1041436057,1.1986032881,-0.5702865518

N,0,-1.2837234082,-0.1151062064,-0.5391453973

C,0,-0.0991820882,-0.0616471327,0.3973885001

C,0,-0.4242382364,0.1636494801,1.8705299527

O,0,0.6838250115,-0.0174759397,2.5806579489

C,0,0.5898649897,0.1993735598,4.0157526232

C,0,-0.7398988833,-0.4236169176,-1.9162443744

C,0,-2.2262237916,-1.2336805852,-0.144542182

O,0,-1.5076707513,0.479203372,2.3247792109

N,0,0.7665520456,6.0322180622,-1.8129667939

O,0,1.207557151,6.7020261,-0.8756016245

O,0,0.9019412626,6.3414188777,-2.9994743762

H,0,-0.9699986997,2.9769552911,1.1625025894

H,0,0.2699065851,5.0549414773,0.6282662507

H,0,-0.3465558286,4.3509670634,-3.5715783714

H,0,-1.5851635796,2.272731162,-3.0479387033

H,0,-2.5570491925,1.2774004535,0.4154611062

H,0,-2.885406996,1.0157413942,-1.3088177431

H,0,-0.0281401163,0.3473777949,-2.2043291296

H,0,-1.5729476591,-0.4568115012,-2.6169536828

H,0,-0.2446072783,-1.3931611564,-1.8827663853

H,0,-3.0036126398,-1.3055444583,-0.9037284675

H,0,-1.6585725259,-2.1625608642,-0.101903772

H,0,-2.6613065068,-1.0046643418,0.8247405898

H,0,0.4400637985,-1.0047893364,0.2935338452

H,0,0.5645889092,0.7363527623,0.0582008917

H,0,-0.1317880724,-0.4958575336,4.4464311047

H,0,1.5905678544,0.0056321592,4.3949929297

H,0,0.2900448096,1.2291853615,4.2142782614

TS B3LYP 23PSPCMDMSO

home/biswas/quiver/tdb3lyp

Nitro TS

b3lyp/6-31+G**

E(RB3LYP) = -877.211171489

Zero-point correction= 0.272537 (Hartree/Particle)

Thermal correction to Energy= 0.290384

Thermal correction to Enthalpy= 0.291328

Thermal correction to Gibbs Free Energy= 0.225662

Sum of electronic and ZPE= -876.938635

Sum of electronic and thermal Energies= -876.920787

Sum of electronic and thermal Enthalpies= -876.919843

Sum of electronic and thermal Free Energies= -876.985510

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.219	66.379	138.207

C,0,-1.0808483729,-0.3725374146,2.1559026633

C,0,-0.9972605276,-0.5122182633,3.5354914391

C,0,0.2418269108,-0.3399550846,4.1614789989

C,0,1.4006413515,-0.0143916192,3.4280442045

C,0,1.3095689252,0.1121742989,2.0568095078

C,0,0.0688474358,-0.0621126243,1.3794165339

C,0,-0.0209401444,-0.0636030153,-0.0399578643

N,0,-0.073370787,-2.1076034171,-0.5319635418

C,0,-0.9102791393,-2.8441331952,0.2735273667

C,0,-0.5318265823,-3.5661534383,1.4497688504

O,0,-1.6385817641,-4.186023621,1.9843800476

C,0,-1.4144308802,-4.9750281669,3.162971459

C,0,1.3769575876,-2.4352332123,-0.5208470133

C,0,-0.5826603842,-1.974389722,-1.9242645275

O,0,0.5869767421,-3.7013788844,1.9611840351

N,0,0.3317513363,-0.4828214456,5.5971629317

O,0,-0.6951989856,-0.7678639444,6.236730675

O,0,1.4362306021,-0.3181954006,6.1427625937

H,0,-2.0448161614,-0.4674706802,1.6688046323

H,0,-1.8729172162,-0.7479051546,4.1271339687

H,0,2.3419698203,0.1269340985,3.9435208781

H,0,2.1978856181,0.3565458644,1.4821324222

H,0,-0.9909604198,0.1274032535,-0.4856731628

H,0,0.8324392134,0.2767890064,-0.6185165863

H,0,1.7707233538,-2.3258691646,0.4850091359

H,0,1.8853665872,-1.7632564734,-1.2112088319

H,0,1.5080933839,-3.470940365,-0.8470462504

H,0,-0.0102345211,-1.2078932447,-2.4463137326

H,0,-0.4706593285,-2.9343270687,-2.4362877448

H,0,-1.6359249385,-1.6958685798,-1.9011266659

H,0,-1.9610838146,-2.8010239477,0.0227528753

H,0,-0.7122408982,-5.7884152874,2.9613099061

H,0,-1.0264484327,-4.3573150217,3.9772569592

H,0,-2.3903065696,-5.3799340647,3.4312428368

SM B971 23PSPCMDMSO

home/biswas/quiver/sdB971

nitro SM

B971/6-31+g**

E(RB971) = -877.460580758

Zero-point correction= 0.290413 (Hartree/Particle)

Thermal correction to Energy= 0.308148

Thermal correction to Enthalpy= 0.309092

Thermal correction to Gibbs Free Energy= 0.243102

Sum of electronic and ZPE= -877.170167

Sum of electronic and thermal Energies= -877.152433

Sum of electronic and thermal Enthalpies= -877.151489

Sum of electronic and thermal Free Energies= -877.217479

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	193.366	66.352	138.887

C,0,-0.8109345347,3.2446017806,0.1331465757

C,0,-0.1155954008,4.4204406816,-0.1538789018

C,0,0.0455265553,4.7875643044,-1.492491918

C,0,-0.4761866988,4.0287143379,-2.5440115474

C,0,-1.1687192293,2.8564272541,-2.2379030625

C,0,-1.3272402718,2.4418816488,-0.9018367791

C,0,-2.1114471404,1.1909064564,-0.5683067559

N,0,-1.286018257,-0.1169961407,-0.5407308391

C,0,-0.0998571637,-0.058500851,0.3925025955

C,0,-0.4267976362,0.1682402201,1.8694850358

O,0,0.6842374482,-0.003110383,2.5759505435

C,0,0.5862343123,0.2194067975,4.0069782269

C,0,-0.7431321947,-0.4193941131,-1.9191991622

C,0,-2.221468805,-1.2407178432,-0.1464412976

O,0,-1.5120121199,0.4772646188,2.3245782023

N,0,0.7764981271,6.0248258274,-1.80590964

O,0,1.2227704611,6.6892671054,-0.8667733083

O,0,0.9084459422,6.3360225136,-2.9926498793

H,0,-0.965106897,2.9638513877,1.1717927294

H,0,0.285522616,5.0429555813,0.6379530136

H,0,-0.3492498814,4.354079392,-3.5703556435

H,0,-1.5980561072,2.2733111002,-3.0480576987

H,0,-2.8930135365,1.008481899,-1.3098868176

H,0,-2.5657048646,1.26818301,0.4195783452

H,0,-0.0335172771,0.357152405,-2.2060049196

H,0,-1.5791090198,-0.4537215782,-2.6195176683

H,0,-0.2432577673,-1.3888472522,-1.8885509189

H,0,0.4435383222,-1.0018134095,0.2892298166

H,0,0.5607863304,0.7445744918,0.0516704191

H,0,-1.6475396985,-2.1680356723,-0.1063309638

H,0,-3.0007411333,-1.3149369722,-0.906301611

H,0,-2.6570204745,-1.0146883958,0.825661192

H,0,-0.1321510406,-0.4798955373,4.4410401879

H,0,1.5889828316,0.0348047607,4.3900456541

H,0,0.2779002037,1.2495075739,4.2010397951

TS B971 23PSPCMDMSO

home/biswas/quiver/tdB971

Nitro TS

B971/6-31+G**

E(RB971) = -876.953613758

Zero-point correction= 0.271946 (Hartree/Particle)

Thermal correction to Energy= 0.289815

Thermal correction to Enthalpy= 0.290759

Thermal correction to Gibbs Free Energy= 0.225323

Sum of electronic and ZPE= -876.681668

Sum of electronic and thermal Energies= -876.663799

Sum of electronic and thermal Enthalpies= -876.662854

Sum of electronic and thermal Free Energies= -876.728291

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 181.862 66.610 137.722

C,0,-1.089893258,-0.4062375304,2.1079001083

C,0,-1.009572898,-0.6002441731,3.4847653808

C,0,0.2262309241,-0.4328047629,4.1240880111

C,0,1.3861738453,-0.0529073392,3.409879865

C,0,1.3003378973,0.1253276253,2.0420868239

C,0,0.0625508737,-0.0458134914,1.3480600784

C,0,-0.0164093387,-0.0234027205,-0.0702791897

N,0,-0.0695891038,-2.1062572591,-0.5345581702

C,0,-0.9024649418,-2.8161227303,0.2917100294

C,0,-0.5154132666,-3.5252808871,1.4838006159

O,0,-1.6239261959,-4.1068756607,2.0458912269

C,0,-1.3974280341,-4.8459776297,3.2538326666

C,0,1.3821731289,-2.4187507852,-0.5156223769

C,0,-0.5837029621,-1.9867425608,-1.9248570469

O,0,0.6092738419,-3.6731294758,1.9742290277

N,0,0.3127509749,-0.6377234396,5.5517708674

O,0,-0.7072422579,-0.9902120935,6.16981362

O,0,1.4081403953,-0.4579104737,6.1120703314

H,0,-2.0529360909,-0.491346401,1.613065255

H,0,-1.8843967631,-0.8757351604,4.0640049118

H,0,2.3227143445,0.08503363,3.9389076417

H,0,2.1881017104,0.4075208171,1.4805532111

H,0,-0.9868822699,0.1496654044,-0.5274132217

H,0,0.8431211358,0.3180218892,-0.6432611377

H,0,1.7727316532,-2.2863654538,0.4913367157

H,0,1.8851358002,-1.7520354313,-1.2180061295

H,0,1.5254244144,-3.4606190655,-0.8234441994

H,0,-0.0119571385,-1.2235333863,-2.4564895425

H,0,-0.4733831109,-2.9532908142,-2.4290516187

H,0,-1.6384719156,-1.7066889312,-1.9001114794

H,0,-1.9574879698,-2.7743452583,0.0489243536

H,0,-0.6867632881,-5.6619127031,3.0871252325

H,0,-1.0163251599,-4.1899962812,4.0441570345

H,0,-2.3723259764,-5.2473224668,3.5367101038

SM APFD 23PSPCMDMSO

home/biswas/quiver/sdAPFD

nitro SM

APFD/6-31+g**

E(RAPFD) = -877.025345859

Zero-point correction= 0.292848 (Hartree/Particle)

Thermal correction to Energy= 0.310309

Thermal correction to Enthalpy= 0.311253

Thermal correction to Gibbs Free Energy= 0.246081

Sum of electronic and ZPE= -876.732498

Sum of electronic and thermal Energies= -876.715037

Sum of electronic and thermal Enthalpies= -876.714093

Sum of electronic and thermal Free Energies= -876.779265

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	194.722	65.570	137.166

C,0,-0.8607494161,3.1521373478,0.1958305895

C,0,-0.1291869126,4.3093859996,-0.0432664701

C,0,0.0832577268,4.6967319823,-1.3628432359

C,0,-0.4220219972,3.9781016913,-2.4422881411

C,0,-1.1510397075,2.8232596461,-2.1843350257

C,0,-1.3599503792,2.3909812958,-0.8688686786

C,0,-2.1508313638,1.1438708199,-0.5903610059

N,0,-1.3211883828,-0.1434136417,-0.5773940758

C,0,-0.1278993442,-0.0603669429,0.3242315506

C,0,-0.4273934696,0.2294757358,1.7854829968

O,0,0.7142839325,0.2180332254,2.4526885279

C,0,0.6339425919,0.5054870839,3.8638555058

C,0,-0.8046339731,-0.4326970829,-1.9540897701

C,0,-2.2237742908,-1.2687378234,-0.1643434479

O,0,-1.5224108467,0.4533259643,2.2598676668

N,0,0.85402107,5.9130037567,-1.625010952

O,0,1.2858611581,6.5357077833,-0.6610881703

O,0,1.0260040798,6.2405232904,-2.7939975373

H,0,-1.0558965897,2.8498612836,1.220388168

H,0,0.2638757253,4.9047262161,0.7724863052

H,0,-0.2524917346,4.3213492692,-3.4560696662

H,0,-1.569882336,2.2649277674,-3.0161764996

H,0,-2.9141038869,0.9793498259,-1.3526608381

H,0,-2.6306456486,1.1950293619,0.3854429728

H,0,-0.1255579107,0.3621029044,-2.2582306429

H,0,-1.6511531906,-0.4925618907,-2.6371617976

H,0,-0.2759122339,-1.384895467,-1.9359935508

H,0,0.4083886493,-1.009188663,0.2510056285

H,0,0.5321317459,0.7219083128,-0.0582879634

H,0,-1.6455631686,-2.1923277747,-0.1617171602

H,0,-3.0342376809,-1.3388638289,-0.8889088935

H,0,-2.6168557697,-1.0614078968,0.8280247284

H,0,0.0058162729,-0.236991969,4.358649347

H,0,1.6580808996,0.4484530033,4.2250773087

H,0,0.2242823816,1.5055264138,4.015575227

TS APFD 23PSPCMDMSO

home/biswas/quiver/tdAPFD

Nitro TS

APFD/6-31+G**

E(RAPFD) = -876.519182271

Zero-point correction= 0.274957 (Hartree/Particle)

Thermal correction to Energy= 0.292256

Thermal correction to Enthalpy= 0.293201

Thermal correction to Gibbs Free Energy= 0.230034

Sum of electronic and ZPE= -876.244225

Sum of electronic and thermal Energies= -876.226926

Sum of electronic and thermal Enthalpies= -876.225982

Sum of electronic and thermal Free Energies= -876.289148

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.394	65.531	132.945

C,0,-1.1518065918,-0.4515019913,2.0114856903

C,0,-1.0579653732,-0.7805573839,3.3567391329

C,0,0.1830064846,-0.6968765294,3.9812379893

C,0,1.3254821615,-0.2200221372,3.3137499984

C,0,1.226020477,0.0940554265,1.9778636077

C,0,-0.0060496,-0.0402515935,1.2853600334

C,0,-0.0736724071,-0.026602385,-0.1297858662

N,0,-0.0464164536,-2.0428842538,-0.507850729

C,0,-0.8604843055,-2.7553846881,0.335352025

C,0,-0.4690197903,-3.3212339701,1.5891952978

O,0,-1.5577941452,-3.908371757,2.1782344182

C,0,-1.3355976636,-4.4584810771,3.4740481597

C,0,1.4031697868,-2.3148493653,-0.4527661033

C,0,-0.5363725523,-2.0249072157,-1.8997312691

O,0,0.6419362106,-3.3452326139,2.1252985497

N,0,0.2979934742,-1.1149280815,5.3558713536

O,0,-0.6847260255,-1.6299609021,5.8971803179

O,0,1.3789936581,-0.955206585,5.9282600825

H,0,-2.1153845158,-0.4938795271,1.5143369046

H,0,-1.9234704796,-1.1229277155,3.9122573219

H,0,2.2661856904,-0.1395637915,3.8458124661

H,0,2.1054836815,0.4291729999,1.4342605582

H,0,-1.0415233188,0.1370566273,-0.5950383647

H,0,0.7809926074,0.3326086819,-0.6978086787

H,0,1.7755817267,-2.0929583796,0.544076782

H,0,1.8991177965,-1.6936477923,-1.1981054889

H,0,1.5734618905,-3.3718906201,-0.6730302676

H,0,0.0120530302,-1.271479869,-2.465823722

H,0,-0.3806946694,-3.0106745839,-2.3464712298

H,0,-1.5996380483,-1.7852404468,-1.908424977

H,0,-1.9082299462,-2.7822188517,0.0677990371

H,0,-0.5452838357,-5.2139373161,3.4536623667

H,0,-1.0654768775,-3.6755496677,4.1895053425

H,0,-2.2815830767,-4.9156876445,3.7648382606

SM B98 23PSPCMDMSO

home/biswas/quiver/sdB98

nitro SM

B98/6-31+g**

E(RB98) = -877.370701432

Zero-point correction= 0.290834 (Hartree/Particle)

Thermal correction to Energy= 0.308532

Thermal correction to Enthalpy= 0.309476

Thermal correction to Gibbs Free Energy= 0.243624

Sum of electronic and ZPE= -877.079867

Sum of electronic and thermal Energies= -877.062170

Sum of electronic and thermal Enthalpies= -877.061226

Sum of electronic and thermal Free Energies= -877.127077

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	193.607	66.227	138.597

C,0,-0.8101148015,3.2488092351,0.1304787905

C,0,-0.1162591809,4.4242394906,-0.1579122534

C,0,0.0443446601,4.7895046354,-1.4962147062

C,0,-0.4767642256,4.0292618783,-2.5459704699

C,0,-1.1677713422,2.857434636,-2.2383780943

C,0,-1.3252259642,2.4442312397,-0.9025515279

C,0,-2.1089100349,1.1934823309,-0.5669349238

N,0,-1.285115622,-0.115420897,-0.5391799474

C,0,-0.1002117189,-0.0595666708,0.3953522593

C,0,-0.4277607231,0.1648055309,1.8722280415

O,0,0.6813673917,-0.0063933634,2.5786635394

C,0,0.5859481254,0.2114322551,4.0093605986

C,0,-0.7409037748,-0.4184331326,-1.9168761273

C,0,-2.2227964543,-1.2381591481,-0.1472526803

O,0,-1.5123719133,0.4716022424,2.3266303916

N,0,0.7738733948,6.0259087737,-1.8112196635

O,0,1.2200157978,6.6914946642,-0.8742924079

O,0,0.9051753949,6.3359312384,-2.9971836196

H,0,-0.9639545103,2.9701489898,1.168963703

H,0,0.2839073414,5.047500753,0.6329428342

H,0,-0.350706421,4.3529377011,-3.5722876945

H,0,-1.5965679868,2.2737645723,-3.0475152744

H,0,-2.8913858868,1.0113492434,-1.3066647349

H,0,-2.5617371599,1.2719013721,0.4208045339

H,0,-0.0293766987,0.3559114626,-2.2024139383

H,0,-1.5752458196,-0.450770372,-2.6182666899

H,0,-0.243551158,-1.3885102378,-1.8860194277

H,0,0.4419592443,-1.0028124052,0.2916000063

H,0,0.5616468413,0.7425488523,0.0567952052

H,0,-1.6502109831,-2.1655038578,-0.1049500403

H,0,-2.9994068474,-1.3122847241,-0.908972273

H,0,-2.6610609972,-1.0118465341,0.8228123352

H,0,-0.1301550463,-0.489825269,4.4425511875

H,0,1.5889823172,0.0271676317,4.3902017622

H,0,0.2769107616,1.2399648829,4.207184306

TS B98 23PSPCMDMSO

home/biswas/quiver/tdB98

Nitro TS

B98/6-31+G**

E(RB98) = -876.863204208

Zero-point correction= 0.272350 (Hartree/Particle)

Thermal correction to Energy= 0.290161

Thermal correction to Enthalpy= 0.291105

Thermal correction to Gibbs Free Energy= 0.225932

Sum of electronic and ZPE= -876.590855

Sum of electronic and thermal Energies= -876.573043

Sum of electronic and thermal Enthalpies= -876.572099

Sum of electronic and thermal Free Energies= -876.637272

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.079	66.474	137.168

C,0,-1.0870624322,-0.3965925174,2.1139567476

C,0,-1.0077320365,-0.5823990058,3.4909983571

C,0,0.2277391239,-0.4151897021,4.1298986812

C,0,1.3887846248,-0.0451911614,3.4133585302

C,0,1.3038895136,0.1259770691,2.0457225109

C,0,0.0658470989,-0.0433957593,1.3522688591

C,0,-0.0134003277,-0.0203058181,-0.0646359117

N,0,-0.0712123432,-2.112409175,-0.5331704321

C,0,-0.9036675073,-2.8204663386,0.2919702825

C,0,-0.5168061357,-3.5362275157,1.4800622004

O,0,-1.6228920477,-4.1206388687,2.0382262416

C,0,-1.3987188603,-4.8735328769,3.2367393396

C,0,1.3801477019,-2.4250216098,-0.5165588238

C,0,-0.5869054539,-1.9861295607,-1.921929996

O,0,0.6069377008,-3.685848703,1.9685648339

N,0,0.31272461,-0.6094999348,5.5573204941

O,0,-0.7086332035,-0.9496454349,6.1782593821

O,0,1.4082440036,-0.4330890018,6.1165203439

H,0,-2.0500275302,-0.4807061635,1.6201688967

H,0,-1.8834768655,-0.8507022237,4.0710178076

H,0,2.3255113813,0.0920254169,3.9409357641

H,0,2.1924750539,0.4018843448,1.4835856195

H,0,-0.9831516102,0.1516443522,-0.5219008917

H,0,0.8461343313,0.3180484746,-0.6380683165

H,0,1.7715242431,-2.2978072215,0.4899721047

H,0,1.8826419223,-1.7556302558,-1.2156954997

H,0,1.5230043891,-3.4648982158,-0.8294940251

H,0,-0.0151342751,-1.2221313205,-2.4510491984

H,0,-0.4786273757,-2.9502329351,-2.4301357803

H,0,-1.6407239062,-1.705064238,-1.8950749058

H,0,-1.9582545437,-2.7780427775,0.0502010496

H,0,-0.6973236305,-5.6942470289,3.0582441027

H,0,-1.0080067608,-4.2301103431,4.0315968834

H,0,-2.3755598525,-5.26843895,3.5197137487

SM B972 23PSPCMDMSO

home/biswas/quiver/sdB972

nitro SM

B972/6-31+g**

E(RB972) = -877.403697476

Zero-point correction= 0.293487 (Hartree/Particle)

Thermal correction to Energy= 0.311097

Thermal correction to Enthalpy= 0.312041

Thermal correction to Gibbs Free Energy= 0.246211

Sum of electronic and ZPE= -877.110211

Sum of electronic and thermal Energies= -877.092600

Sum of electronic and thermal Enthalpies= -877.091656

Sum of electronic and thermal Free Energies= -877.157486

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	195.216	65.769	138.551

C,0,-0.7883040311,3.2429406879,0.1210373043

C,0,-0.101131406,4.4146568482,-0.1740851218

C,0,0.0393618476,4.7832125343,-1.5082679381

C,0,-0.4974809566,4.0284121784,-2.5469203029

C,0,-1.1816453511,2.8602165352,-2.2329909713

C,0,-1.3177062078,2.4434383505,-0.9014868984

C,0,-2.0945195038,1.198268728,-0.5613055409

N,0,-1.2781315536,-0.1043165954,-0.5326877483

C,0,-0.1071515003,-0.0520883547,0.406679639

C,0,-0.4386988165,0.1574639918,1.8763804902

O,0,0.6682695054,-0.0112561708,2.5810823271

C,0,0.5701167987,0.1919873894,4.0079206857

C,0,-0.7264483841,-0.4014953549,-1.8995018342

C,0,-2.2137516121,-1.2223225378,-0.1539650779

O,0,-1.5234715995,0.4513700113,2.3302324584

N,0,0.7639414572,6.0174839912,-1.8302220821

O,0,1.2173631517,6.674830385,-0.9035578482

O,0,0.8786229865,6.3242301671,-3.0088258564

H,0,-0.9254492491,2.9643115019,1.1588628108

H,0,0.3097965823,5.0335327553,0.6109806365

H,0,-0.3887507756,4.3530011152,-3.5720738421

H,0,-1.6224912578,2.2813364502,-3.035339204

H,0,-2.8787745191,1.0175855162,-1.2949372579

H,0,-2.5457191496,1.2795945059,0.4237398089

H,0,-0.0115645111,0.3681836382,-2.1768192181

H,0,-1.5511984442,-0.4289027573,-2.6072953737

H,0,-0.233770221,-1.3703091765,-1.8703010238

H,0,0.4394606687,-0.9885685156,0.2988735675

H,0,0.5540214035,0.7510517243,0.0799026686

H,0,-1.6441285522,-2.1474548744,-0.1082676349

H,0,-2.9818715894,-1.2970319772,-0.9194761802

H,0,-2.6601571104,-1.0008438075,0.8098316327

H,0,-0.1369168777,-0.5173605754,4.4347312123

H,0,1.5714227961,0.013960043,4.3875583427

H,0,0.2534219822,1.212688649,4.2160263703

TS B972 23PSPCMDMSO

home/biswas/quiver/tdB972

Nitro TS

B972/6-31+G**

E(RB972) = -876.893771677

Zero-point correction= 0.275027 (Hartree/Particle)

Thermal correction to Energy= 0.292722

Thermal correction to Enthalpy= 0.293667

Thermal correction to Gibbs Free Energy= 0.228533

Sum of electronic and ZPE= -876.618745

Sum of electronic and thermal Energies= -876.601049

Sum of electronic and thermal Enthalpies= -876.600105

Sum of electronic and thermal Free Energies= -876.665239

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.686	65.949	137.086

C,0,-1.0762146813,-0.380007967,2.1203188788

C,0,-1.0034208121,-0.5447394702,3.4957258282

C,0,0.2257207897,-0.3794159079,4.1349468583

C,0,1.3871022844,-0.0343896491,3.4187048577

C,0,1.3082163795,0.1186051571,2.0528322265

C,0,0.0761755374,-0.0466239562,1.3604061229

C,0,-0.000733818,-0.0290663692,-0.052329847

N,0,-0.073349101,-2.1115933453,-0.5208193904

C,0,-0.8998265385,-2.815891984,0.3060768274

C,0,-0.5122518395,-3.549827442,1.4750368779

O,0,-1.6174939694,-4.1383848814,2.0236208139

C,0,-1.392784103,-4.9296068573,3.1900630434

C,0,1.3681297826,-2.432197601,-0.5172278994

C,0,-0.597073782,-1.9843665198,-1.8980601955

O,0,0.6088285716,-3.7120956927,1.9573355141

N,0,0.303622417,-0.5499330495,5.5646230381

O,0,-0.718331616,-0.8580169478,6.1805129622

O,0,1.3926895575,-0.3838388077,6.1166391485

H,0,-2.0362619615,-0.4629819866,1.6265781773

H,0,-1.8825729515,-0.7948266351,4.0736019492

H,0,2.3223035749,0.101178558,3.9438869634

H,0,2.1994205959,0.3786906359,1.4926823783

H,0,-0.9657230131,0.1537492852,-0.5086388397

H,0,0.8592790838,0.3025639871,-0.6234732879

H,0,1.7726001089,-2.301521983,0.4800203721

H,0,1.8679665666,-1.7732447827,-1.2230764548

H,0,1.5025702802,-3.4713603465,-0.8244523742

H,0,-0.0279524481,-1.2271897518,-2.4332481867

H,0,-0.4998864333,-2.9463282985,-2.4056497087

H,0,-1.6459550931,-1.6981752213,-1.865158274

H,0,-1.9524736486,-2.7686220558,0.0702870298

H,0,-0.7189918973,-5.7607367549,2.9756108858

H,0,-0.9737207924,-4.3255679871,3.9964416189

H,0,-2.3713180304,-5.3082503716,3.4777710854

SM MN12SX 23PSPCMDMSO

home/biswas/quiver/sdMN12SX

nitro SM

MN12SX/6-31+g**

E(RMN12SX) = -877.004565778

Zero-point correction= 0.292088 (Hartree/Particle)

Thermal correction to Energy= 0.309594

Thermal correction to Enthalpy= 0.310538

Thermal correction to Gibbs Free Energy= 0.245300

Sum of electronic and ZPE= -876.712477

Sum of electronic and thermal Energies= -876.694972

Sum of electronic and thermal Enthalpies= -876.694028

Sum of electronic and thermal Free Energies= -876.759266

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 194.273 65.679 137.304

C,0,-0.8675696625,3.1779217069,0.1836871899

C,0,-0.1445896564,4.3380071066,-0.0605687509

C,0,0.072611936,4.7099121417,-1.3824212398

C,0,-0.4157596504,3.9783111842,-2.4594463138

C,0,-1.1343104779,2.8203424469,-2.1938401396

C,0,-1.3502888729,2.4002837179,-0.8760305028

C,0,-2.1438492571,1.1544786817,-0.5886897255

N,0,-1.3163632033,-0.1304002241,-0.5627634098

C,0,-0.1191058795,-0.0574429589,0.3312967706

C,0,-0.4109011551,0.2205013572,1.7927276226

O,0,0.7201166708,0.1782374674,2.4674926659

C,0,0.6332103684,0.4453955687,3.8749915319

C,0,-0.8027512658,-0.4316515523,-1.9388549021

C,0,-2.2254719891,-1.2508092001,-0.1499743218

O,0,-1.497735266,0.461688073,2.2685002292

N,0,0.8311955343,5.9261559199,-1.6495656745

O,0,1.2815667489,6.5491302223,-0.6922822259

O,0,0.9850935228,6.2669746336,-2.818823467

H,0,-1.0739018337,2.8857708734,1.2142863679

H,0,0.2365176493,4.9489396248,0.7540225673

H,0,-0.2414887771,4.3139404977,-3.4788527585

H,0,-1.5441400102,2.248572617,-3.0266440153

H,0,-2.9041162507,0.9829453873,-1.360157997

H,0,-2.6383142599,1.2191816636,0.3846420961

H,0,-0.0945351684,0.3447290758,-2.2412257671

H,0,-1.6511345898,-0.4693585365,-2.628408996

H,0,-0.2990051265,-1.4022449324,-1.9188708771

H,0,0.4151566362,-1.0125588216,0.250210348

H,0,0.5530222352,0.7229722217,-0.0491729223

H,0,-1.6440579539,-2.1769505748,-0.1190291222

H,0,-3.0205500794,-1.3353028237,-0.8964439921

H,0,-2.649182586,-1.0296685654,0.8314670227

H,0,-0.0109880735,-0.2980223695,4.3561325687

H,0,1.6555089124,0.3705743076,4.2485017593

H,0,0.2326768307,1.451251062,4.039621381

TS MN12SX 23PSPCMDMSO

home/biswas/quiver/tdMN12SX

Nitro TS

MN12SX/6-31+G**

E(RMN12SX) = -876.505223838

Zero-point correction= 0.274467 (Hartree/Particle)

Thermal correction to Energy= 0.291727

Thermal correction to Enthalpy= 0.292671

Thermal correction to Gibbs Free Energy= 0.229848

Sum of electronic and ZPE= -876.230757

Sum of electronic and thermal Energies= -876.213497

Sum of electronic and thermal Enthalpies= -876.212553

Sum of electronic and thermal Free Energies= -876.275376

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.061	65.633	132.222

C,0,-1.1448017133,-0.459572263,2.0430183093

C,0,-1.0530887236,-0.7702425579,3.3899586808

C,0,0.1903578025,-0.6836365285,4.01241842

C,0,1.337761616,-0.233819561,3.3363378528

C,0,1.2385306772,0.0571602901,1.9967201137

C,0,0.0040685451,-0.0741532037,1.3057154787

C,0,-0.0684285296,-0.0420483717,-0.1078706076

N,0,-0.0513316497,-2.0726732142,-0.5289161835

C,0,-0.8699478439,-2.7931306855,0.2959663893

C,0,-0.4862719962,-3.3546189387,1.552444788

O,0,-1.5651877845,-3.9285288875,2.1514731536

C,0,-1.3408002022,-4.4450908523,3.4534407501

C,0,1.3994409127,-2.3293017779,-0.479377049

C,0,-0.541542803,-2.0055256655,-1.9176075412

O,0,0.6234584569,-3.3829124225,2.0830716951

N,0,0.2990580238,-1.0610075715,5.3926987041

O,0,-0.6915177952,-1.5384888449,5.9588348788

O,0,1.3839803247,-0.9095931014,5.9649078444

H,0,-2.1125231008,-0.5038070272,1.5446732313

H,0,-1.9258312504,-1.0893466636,3.9560581387

H,0,2.2820247024,-0.1486551042,3.868052121

H,0,2.1226225708,0.3804490095,1.4456395334

H,0,-1.0409633186,0.1200927716,-0.5729419672

H,0,0.7912576953,0.311960683,-0.679645083

H,0,1.7909675418,-2.0903524644,0.5113256163

H,0,1.8815756516,-1.7114667279,-1.2424885582

H,0,1.5833142054,-3.3908978993,-0.6896588111

H,0,0.0040468316,-1.2262440849,-2.4584488567

H,0,-0.3797202568,-2.9760248915,-2.404601721

H,0,-1.6105463607,-1.773266797,-1.9164997579

H,0,-1.9227076607,-2.8022643678,0.0313398851

H,0,-0.5686860377,-5.2240503577,3.4455141398

H,0,-1.0343443172,-3.6451837215,4.1435855956

H,0,-2.2959352137,-4.8677731994,3.7764498167

SM wB97X 23PSPCMDMSO

home/biswas/quiver/sdwB97X

nitro SM

wB97X/6-31+g**

E(RwB97X) = -877.500265001

Zero-point correction= 0.295999 (Hartree/Particle)

Thermal correction to Energy= 0.313225

Thermal correction to Enthalpy= 0.314169

Thermal correction to Gibbs Free Energy= 0.249716

Sum of electronic and ZPE= -877.204266

Sum of electronic and thermal Energies= -877.187040

Sum of electronic and thermal Enthalpies= -877.186096

Sum of electronic and thermal Free Energies= -877.250549

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	196.552	64.802	135.653

C,0,-0.8369678213,3.182534265,0.1709521955

C,0,-0.1291893687,4.3512472226,-0.0811443422

C,0,0.0649552519,4.729288754,-1.4023452666

C,0,-0.4294951392,3.9952695949,-2.4717556224

C,0,-1.1351555943,2.8298044294,-2.2003813349

C,0,-1.3290432677,2.4045847095,-0.8821902071

C,0,-2.1241434777,1.1573340047,-0.5846595422

N,0,-1.309564243,-0.1349979239,-0.5638958051

C,0,-0.1184435877,-0.0741648598,0.3431753785

C,0,-0.417932501,0.2031404791,1.8065457871

O,0,0.7111388375,0.1418278949,2.4900311985

C,0,0.61838338,0.4127903282,3.9055625154

C,0,-0.7919064148,-0.4391683686,-1.9397326028

C,0,-2.2308685118,-1.2490956323,-0.1531046783

O,0,-1.5057930503,0.459375229,2.2773127049

N,0,0.8108139072,5.967015839,-1.6803279575

O,0,1.2292291775,6.6095581896,-0.7306068814

O,0,0.9741463977,6.2876619145,-2.8467131224

H,0,-1.0204434314,2.8878165454,1.2010110807

H,0,0.2559806555,4.9607476379,0.7277092274

H,0,-0.2732740623,4.3337610977,-3.4891716362

H,0,-1.5483699824,2.2597434232,-3.0276174844

H,0,-2.8945043182,0.9957050029,-1.3411917762

H,0,-2.5996889071,1.2271126573,0.3925528598

H,0,-0.0886950993,0.3360891694,-2.2420133823

H,0,-1.6363156801,-0.4789359988,-2.6279224776

H,0,-0.2890572907,-1.4057790972,-1.9156730657

H,0,0.4040129352,-1.030733424,0.2667680947

H,0,0.556986867,0.7012738797,-0.0265341272

H,0,-1.6634350638,-2.1797401869,-0.135746463

H,0,-3.0332228785,-1.3152914301,-0.8877144222

H,0,-2.6352127712,-1.0289984321,0.8327507528

H,0,-0.0378106626,-0.3193661398,4.3782322275

H,0,1.6350501586,0.3224965749,4.2809836097

H,0,0.234401557,1.4218996506,4.0623675654

TS wB97X 23PSPCMDMSO

home/biswas/quiver/tdwB97X

Nitro TS

wB97X/6-31+G**

E(RwB97X) = -876.971748349

Zero-point correction= 0.277305 (Hartree/Particle)

Thermal correction to Energy= 0.294431

Thermal correction to Enthalpy= 0.295375

Thermal correction to Gibbs Free Energy= 0.232756

Sum of electronic and ZPE= -876.694443

Sum of electronic and thermal Energies= -876.677317

Sum of electronic and thermal Enthalpies= -876.676373

Sum of electronic and thermal Free Energies= -876.738993

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	184.758	65.137	131.794

C,0,-1.1133039754,-0.440839874,1.9425259096

C,0,-1.0529487634,-0.7851007258,3.2919320998

C,0,0.1633970299,-0.714874762,3.9486148939

C,0,1.3306642003,-0.2355802428,3.3144253301

C,0,1.2671670533,0.1100025165,1.9918910406

C,0,0.045279092,0.0096888494,1.2531175828

C,0,0.0109234602,0.1062781203,-0.14256395

N,0,-0.065910799,-2.0932983222,-0.4988891411

C,0,-0.8747081315,-2.6814257147,0.4066946631

C,0,-0.460933154,-3.3342337809,1.6280898145

O,0,-1.5433458277,-3.8780351129,2.2411406868

C,0,-1.2998298907,-4.4996623818,3.5063335073

C,0,1.3805385893,-2.3670072874,-0.4724266679

C,0,-0.6109704543,-2.0378706486,-1.8677300138

O,0,0.667078612,-3.4387651296,2.0986960405

N,0,0.2365405155,-1.1315078899,5.3329108925

O,0,-0.7486120646,-1.6599883689,5.8430396602

O,0,1.2859705748,-0.9531761745,5.9441189831

H,0,-2.0753020189,-0.4299988269,1.4399491118

H,0,-1.9370929609,-1.1264683393,3.8194346668

H,0,2.2569660258,-0.1672532038,3.8733160976

H,0,2.1603429524,0.4649535385,1.483261136

H,0,-0.9440082635,0.2464080179,-0.6407256247

H,0,0.8924795403,0.4379986835,-0.6867972733

H,0,1.7913134751,-2.0919595178,0.49712773

H,0,1.8510958314,-1.7846054082,-1.26465587

H,0,1.5507873984,-3.4344794248,-0.6441287729

H,0,-0.0505977025,-1.3052520266,-2.4490627525

H,0,-0.5219856116,-3.0258019902,-2.3307503399

H,0,-1.6610703862,-1.7465924689,-1.8294378937

H,0,-1.9302457659,-2.7069874584,0.1667029081

H,0,-0.5622301063,-5.2996911761,3.4099092204

H,0,-0.9487726422,-3.7620526263,4.2349683391

H,0,-2.2603868319,-4.9068358431,3.8205569851

SM B3LYPD2 23PSPCMDMSO

home/biswas/quiver/sdb3lypd2

nitro SM

b3lyp/6-31+g**

E(RB3LYP) = -877.768664815

Zero-point correction= 0.290909 (Hartree/Particle)

Thermal correction to Energy= 0.308362

Thermal correction to Enthalpy= 0.309306

Thermal correction to Gibbs Free Energy= 0.244291

Sum of electronic and ZPE= -877.477756

Sum of electronic and thermal Energies= -877.460303

Sum of electronic and thermal Enthalpies= -877.459359

Sum of electronic and thermal Free Energies= -877.524374

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	193.500	65.862	136.836

C,0,-0.8749966151,3.1504828346,0.1971577289

C,0,-0.1363626458,4.3078336788,-0.0378850331

C,0,0.0861358561,4.6963426002,-1.3600776549

C,0,-0.4139572222,3.9743137368,-2.4452496889

C,0,-1.1501594257,2.8196291795,-2.1901962703

C,0,-1.3733465381,2.3915447083,-0.8729938152

C,0,-2.1718220475,1.1457074604,-0.5979737295

N,0,-1.3276277305,-0.1434041375,-0.5792947116

C,0,-0.124345857,-0.054577329,0.3223298619

C,0,-0.420411959,0.2396958406,1.7869288225

O,0,0.7241674587,0.2151224233,2.458737545

C,0,0.6483920349,0.5062745915,3.8829336992

C,0,-0.8114608492,-0.4333903281,-1.9674126602

C,0,-2.2289333939,-1.2818213923,-0.1622080463

O,0,-1.5133341391,0.4775257686,2.2651781236

N,0,0.8652951107,5.9172546873,-1.6193728126

O,0,1.2967774794,6.5494308045,-0.6517378254

O,0,1.0515806679,6.2510959127,-2.7923917499

H,0,-1.0759785112,2.8429268212,1.2176124879

H,0,0.2536497583,4.9000112621,0.7799554386

H,0,-0.2351938698,4.3133302672,-3.4575143007

H,0,-1.5607177391,2.256454862,-3.0211827847

H,0,-2.6534040598,1.194594962,0.3758862358

H,0,-2.9208400733,0.9721689854,-1.3717243032

H,0,-0.1443694916,0.3723291217,-2.2705385883

H,0,-1.6681205317,-0.5011447686,-2.6380428099

H,0,-0.274243775,-1.381510057,-1.9400469694

H,0,-3.0349298303,-1.350712854,-0.8931531893

H,0,-1.6370203552,-2.1977807934,-0.1602824122

H,0,-2.6222685654,-1.067514956,0.8291302722

H,0,0.4058898307,-1.0062260178,0.2470061506

H,0,0.5283269205,0.729227281,-0.0673449007

H,0,0.0087939375,-0.2318056955,4.3717981769

H,0,1.6746992924,0.4368057845,4.2396065178

H,0,0.2467028785,1.5115897554,4.0278781954

TS B3LYPD2 23PSPCMDMSO

home/biswas/quiver/tdb3lypd2

Nitro TS

b3lyp/6-31+G**

E(RB3LYP) = -877.263539919

Zero-point correction= 0.273043 (Hartree/Particle)

Thermal correction to Energy= 0.290382

Thermal correction to Enthalpy= 0.291327

Thermal correction to Gibbs Free Energy= 0.227895

Sum of electronic and ZPE= -876.990497

Sum of electronic and thermal Energies= -876.973157

Sum of electronic and thermal Enthalpies= -876.972213

Sum of electronic and thermal Free Energies= -877.035645

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.218	65.773	133.502

C,0,-1.1549491543,-0.4765755152,2.0403701143

C,0,-1.0526303134,-0.7892901695,3.3909478799

C,0,0.192400772,-0.6787886023,4.0136853946

C,0,1.3300267575,-0.2016383486,3.3317146261

C,0,1.2221366874,0.0848049189,1.9856671932

C,0,-0.0139739615,-0.06898082,1.3028268946

C,0,-0.0918598709,-0.0674274847,-0.1203107342

N,0,-0.043111992,-2.0340776439,-0.5271643537

C,0,-0.8616416264,-2.7882192502,0.2967462981

C,0,-0.4808775577,-3.3520678074,1.5503850145

O,0,-1.5764244326,-3.9426326245,2.1474720479

C,0,-1.3596681912,-4.4559092724,3.4711245922

C,0,1.4194868576,-2.2976634584,-0.4719774122

C,0,-0.5218711513,-2.0102101492,-1.9357404878

O,0,0.6310193314,-3.3818599224,2.0943333009

N,0,0.3159406703,-1.0756097861,5.4021669706

O,0,-0.6555526496,-1.6167496808,5.9556035042

O,0,1.3936306398,-0.8767027734,5.9851388214

H,0,-2.1150719047,-0.5480213222,1.5431981392

H,0,-1.9111537465,-1.1365145848,3.9514977883

H,0,2.2718726121,-0.1035439867,3.8561795373

H,0,2.0963987241,0.4106480219,1.430436405

H,0,-1.0641086354,0.1066096062,-0.5717806656

H,0,0.7589754586,0.2978161739,-0.689003865

H,0,1.781868034,-2.0875000631,0.5310317363

H,0,1.9045630821,-1.6534352793,-1.2063983104

H,0,1.5936450858,-3.3501053615,-0.7124997099

H,0,0.0314072968,-1.2447427894,-2.4822666844

H,0,-0.3495733175,-2.9934059313,-2.3830378719

H,0,-1.5878317456,-1.7778708324,-1.9450075668

H,0,-1.9081317529,-2.7956940146,0.0253215931

H,0,-0.5614267168,-5.2045361372,3.4751805202

H,0,-1.0978091626,-3.6442342642,4.1591280171

H,0,-2.3074151268,-4.909885845,3.766620273

SM PBE0 23PSPCMDMSO

home/biswas/quiver/sdPBE1PBE

nitro SM

PBE1PBE/6-31+g**

E(RPBE1PBE) = -876.724160272

Zero-point correction= 0.293397 (Hartree/Particle)

Thermal correction to Energy= 0.310924

Thermal correction to Enthalpy= 0.311868

Thermal correction to Gibbs Free Energy= 0.246374

Sum of electronic and ZPE= -876.430763

Sum of electronic and thermal Energies= -876.413236

Sum of electronic and thermal Enthalpies= -876.412292

Sum of electronic and thermal Free Energies= -876.477786

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	195.108	65.554	137.845

C,0,-0.7815864748,3.2182191625,0.1334902019

C,0,-0.0888628886,4.3863752461,-0.1583182437

C,0,0.0444512134,4.760203653,-1.4903443897

C,0,-0.5009076478,4.0171058065,-2.5310839119

C,0,-1.1902295149,2.8520712221,-2.220637002

C,0,-1.321782182,2.4310878483,-0.8913981658

C,0,-2.0978556578,1.1878050223,-0.5552765614

N,0,-1.2766950456,-0.1028407483,-0.5368999999

C,0,-0.1030184771,-0.0418484619,0.389798123

C,0,-0.4337813331,0.1716403995,1.8545976963

O,0,0.6699976605,0.0189793159,2.5633792397

C,0,0.5536971393,0.2324203412,3.9830503176

C,0,-0.7363539737,-0.390046127,-1.9043580502

C,0,-2.1974507099,-1.2237578514,-0.1523921229

O,0,-1.5220894635,0.4583243272,2.305482046

N,0,0.7714671573,5.9891787425,-1.8079734399

O,0,1.2346103616,6.6366867052,-0.8798849132

O,0,0.8786940196,6.3028888556,-2.9849003348

H,0,-0.916283421,2.9308262723,1.1719809238

H,0,0.3331340974,5.0018288877,0.626949077

H,0,-0.3929220549,4.3511606704,-3.5558759892

H,0,-1.6402272356,2.276803351,-3.0237973469

H,0,-2.8852474982,1.0082116821,-1.2898107006

H,0,-2.5463838559,1.2636553182,0.4347088167

H,0,-0.0306637614,0.389971643,-2.1871984889

H,0,-1.5692571493,-0.4242416644,-2.6063126518

H,0,-0.2321148899,-1.3559545539,-1.882325532

H,0,0.4508238016,-0.9774790286,0.2829170087

H,0,0.5532758206,0.7670172129,0.0572317532

H,0,-1.6210757102,-2.1481318319,-0.1171512988

H,0,-2.9763791363,-1.3001077059,-0.9105156297

H,0,-2.6341365682,-1.0068304109,0.8200261728

H,0,-0.1529753697,-0.4813791778,4.4090857642

H,0,1.5533453932,0.0690245827,4.3793351022

H,0,0.221349355,1.2529382939,4.1799355301

TS PBE0 23PSPCMDMSO

home/biswas/quiver/tdPBE1PBE

Nitro TS

PBE1PBE/6-31+G**

E(RPBE1PBE) = -876.214648000

Zero-point correction= 0.274932 (Hartree/Particle)

Thermal correction to Energy= 0.292553

Thermal correction to Enthalpy= 0.293497

Thermal correction to Gibbs Free Energy= 0.228901

Sum of electronic and ZPE= -875.939716

Sum of electronic and thermal Energies= -875.922095

Sum of electronic and thermal Enthalpies= -875.921151

Sum of electronic and thermal Free Energies= -875.985747

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 183.580 65.866 135.953

C,0,-1.0869492893,-0.4314798058,2.0386334655

C,0,-1.0167271336,-0.6794469928,3.4021838315

C,0,0.2044418534,-0.532901447,4.0541666759

C,0,1.3622739944,-0.1108934098,3.372941679

C,0,1.2887204267,0.1230386175,2.0211561139

C,0,0.0646274517,-0.029317693,1.3096360256

C,0,0.0025492801,0.0240596426,-0.0951842772

N,0,-0.0711896744,-2.0953583953,-0.5083704773

C,0,-0.8943682772,-2.7502349191,0.3496542653

C,0,-0.49913853,-3.4441946003,1.5432389834

O,0,-1.5963495792,-4.0085498583,2.1188381851

C,0,-1.3596414335,-4.7410055314,3.3174588867

C,0,1.3681714271,-2.3968740549,-0.4820789696

C,0,-0.5927898156,-2.0010241738,-1.8825887813

O,0,0.6249317652,-3.5880745683,2.0194893407

N,0,0.2795964814,-0.8019447455,5.4643081495

O,0,-0.7325178975,-1.1936143758,6.0473041566

O,0,1.3578473764,-0.6348469782,6.0359268307

H,0,-2.046824763,-0.4865812758,1.5361181349

H,0,-1.8927832988,-0.9851331802,3.9623543534

H,0,2.2906989864,0.0119316645,3.9178418766

H,0,2.1770919598,0.4375936368,1.4803319431

H,0,-0.9613596245,0.1808985884,-0.5689944463

H,0,0.8706956955,0.35531592,-0.6589958048

H,0,1.7660111575,-2.2118229182,0.5128548377

H,0,1.8645230387,-1.7663159697,-1.2192517812

H,0,1.519447938,-3.4508382517,-0.7354506982

H,0,-0.0210233572,-1.2554842405,-2.435712173

H,0,-0.4976739805,-2.9764208787,-2.3702895132

H,0,-1.6431925592,-1.7105780205,-1.856447961

H,0,-1.9492579565,-2.7275934856,0.1089110192

H,0,-0.6542109355,-5.5581041579,3.1447502208

H,0,-0.9679063924,-4.0881150221,4.1026053251

H,0,-2.3294353344,-5.1401041198,3.6142495828

SM M062XD3 23PSPCMDMSO

home/biswas/quiver/sdm062xd3

nitro SM

m062x/6-31+g**

E(RM062X) = -877.336386670

Zero-point correction= 0.294298 (Hartree/Particle)

Thermal correction to Energy= 0.311647

Thermal correction to Enthalpy= 0.312591

Thermal correction to Gibbs Free Energy= 0.247235

Sum of electronic and ZPE= -877.042088

Sum of electronic and thermal Energies= -877.024740

Sum of electronic and thermal Enthalpies= -877.023796

Sum of electronic and thermal Free Energies= -877.089151

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	195.561	65.154	137.552

C,0,-0.1229617256,-0.0842395845,0.2955138242

C,0,-0.4086360795,0.2314785413,1.7535147548

H,0,0.3879903527,-1.0484508192,0.2364750723

H,0,0.5505118298,0.6779427822,-0.1033517028

O,0,-1.5008839838,0.4165761703,2.2407352467

O,0,0.7360628645,0.2888143628,2.410141789

C,0,0.6453987791,0.6007968591,3.8149575311

H,0,1.6701127361,0.5984692237,4.1762612885

H,0,0.1897383386,1.5835324451,3.9417596776

H,0,0.0497656418,-0.1586761737,4.3220653311

N,0,-1.3321795593,-0.1568837502,-0.5863853593

C,0,-0.8377659991,-0.4487725744,-1.9756066474

C,0,-2.2350049617,-1.2845112051,-0.1630898212

H,0,-1.6965749966,-0.4878962233,-2.6451878039

H,0,-0.1457261293,0.3346751856,-2.2810158453

H,0,-0.3292131556,-1.4120908005,-1.9640905425

H,0,-3.0458160925,-1.3539058195,-0.8876050943

H,0,-1.6525404001,-2.2054782126,-0.1622684823

H,0,-2.6234843717,-1.0711498523,0.8297528606

C,0,-2.1584296139,1.1314004373,-0.586396045

H,0,-2.9171957178,0.9797422259,-1.3561264184

C,0,-1.3538160991,2.3770512297,-0.852458427

C,0,-0.8729521768,3.1363427271,0.2208645482

C,0,-0.1383086207,4.2948522046,-0.0046449049

C,0,0.0921668451,4.6772876036,-1.3196643281

C,0,-0.3906480241,3.9643663492,-2.4095508815

C,0,-1.1252173352,2.8102896985,-2.1633774517

H,0,-1.0880485307,2.8356638294,1.24224008

H,0,0.2400546529,4.8923681793,0.8153505525

N,0,0.8689136722,5.9029725957,-1.5691486809

H,0,-0.2038359517,4.3102065205,-3.4184574876

H,0,-1.5339478377,2.2555880741,-3.0023447555

H,0,-2.6410172208,1.1792599168,0.3882123268

O,0,1.0848761204,6.2146473918,-2.7276846783

O,0,1.2551787501,6.5395374618,-0.6038765256

TS M062XD3 23PSPCMDMSO

home/biswas/quiver/tdm062xd3

Nitro TS

m062x/6-31+G**

E(RM062X) = -876.824570553

Zero-point correction= 0.275768 (Hartree/Particle)

Thermal correction to Energy= 0.293008

Thermal correction to Enthalpy= 0.293952

Thermal correction to Gibbs Free Energy= 0.231054

Sum of electronic and ZPE= -876.548802

Sum of electronic and thermal Energies= -876.531562

Sum of electronic and thermal Enthalpies= -876.530618

Sum of electronic and thermal Free Energies= -876.593517

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.865	65.422	132.382

C,0,-1.1350913442,-0.4659555781,1.9542508634

C,0,-1.0594110013,-0.8255239441,3.2966923945

C,0,0.1700126911,-0.7597260033,3.9362435033

C,0,1.3280809572,-0.2692005583,3.2979777862

C,0,1.2465402018,0.0913609868,1.9779366977

C,0,0.0182959297,-0.0138493786,1.2550870531

C,0,-0.0284032739,0.0749668143,-0.1433111227

N,0,-0.0615237822,-2.080953086,-0.5021415026

C,0,-0.8766803074,-2.700982704,0.3776723526

C,0,-0.4700206198,-3.3000088105,1.6272300021

O,0,-1.5502557323,-3.8522645025,2.2393335966

C,0,-1.3063900827,-4.4184022141,3.5271823927

C,0,1.3904647537,-2.3350236119,-0.4441482071

C,0,-0.5740138441,-2.0321784687,-1.8858884437

O,0,0.6489777666,-3.3585881452,2.12297345

N,0,0.2625238589,-1.1940372095,5.3137878408

O,0,-0.7352393225,-1.6679338129,5.8502476836

O,0,1.3397764184,-1.083187598,5.889943848

H,0,-2.0977877936,-0.4673831913,1.4539526262

H,0,-1.9331994845,-1.1774374686,3.8332881493

H,0,2.2586910103,-0.2040533419,3.8480501483

H,0,2.1307468212,0.4535635214,1.4605931527

H,0,-0.9884098941,0.2022099075,-0.6339872468

H,0,0.8457368151,0.4107824052,-0.6952991667

H,0,1.7742081404,-2.0491650366,0.5327570406

H,0,1.8652997851,-1.7510073705,-1.2316233488

H,0,1.57189547,-3.4017136917,-0.6056622413

H,0,-0.0168751166,-1.2813600245,-2.4455192844

H,0,-0.4458798076,-3.015529118,-2.3475608227

H,0,-1.6313664333,-1.7689294442,-1.8681189431

H,0,-1.9277816353,-2.7387685011,0.1237735788

H,0,-0.5426992104,-5.196613075,3.469175298

H,0,-0.9852729142,-3.6439101445,4.2302336293

H,0,-2.2566600194,-4.8432126015,3.846466242

SM M062X 23PSPCMDMSO

home/biswas/quiver/sdm062x

nitro SM

m062x/6-31+g**

E(RM062X) = -877.334180376

Zero-point correction= 0.294303 (Hartree/Particle)

Thermal correction to Energy= 0.311618

Thermal correction to Enthalpy= 0.312562

Thermal correction to Gibbs Free Energy= 0.247625

Sum of electronic and ZPE= -877.039878

Sum of electronic and thermal Energies= -877.022562

Sum of electronic and thermal Enthalpies= -877.021618

Sum of electronic and thermal Free Energies= -877.086555

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	195.543	65.168	136.672

C,0,-0.8590705156,3.1526099243,0.2032767597

C,0,-0.1316177802,4.3131688126,-0.0347238254

C,0,0.0819384935,4.6918893688,-1.3536596229

C,0,-0.4097181784,3.9728257911,-2.4354832546

C,0,-1.1368622763,2.8167974541,-2.176829596

C,0,-1.3497709727,2.3881372412,-0.8618023592

C,0,-2.149980553,1.1426148447,-0.5823519393

N,0,-1.3216376681,-0.1442583944,-0.576678164

C,0,-0.1169112759,-0.0701096798,0.3111206801

C,0,-0.4110549377,0.224977751,1.7716764647

O,0,0.7257579444,0.2268179249,2.4442995608

C,0,0.6288948537,0.520542213,3.8525448645

C,0,-0.82037232,-0.4369329965,-1.9632052783

C,0,-2.2250528898,-1.2720382873,-0.1558158466

O,0,-1.5021932775,0.4419715693,2.2479862701

N,0,0.849895776,5.9203411358,-1.6165948485

O,0,1.2427467547,6.5633900877,-0.6583067375

O,0,1.0523986874,6.2277861649,-2.77869843

H,0,-1.0604935429,2.8533767007,1.227902539

H,0,0.2539746792,4.9153297675,0.7784823609

H,0,-0.2353915726,4.3160358157,-3.4475266165

H,0,-1.5519381423,2.2565053448,-3.0089477563

H,0,-2.6281419289,1.1964076172,0.3940641248

H,0,-2.9117436336,0.9834314775,-1.3475349495

H,0,-0.1248222263,0.3450884352,-2.2642963327

H,0,-1.6754993095,-0.473915156,-2.6376099509

H,0,-0.3145116123,-1.4015941527,-1.9491741075

H,0,-3.030216078,-1.3463819562,-0.8860189752

H,0,-2.6221879349,-1.0553675209,0.8329314099

H,0,-1.6407068126,-2.1917815968,-0.1460019948

H,0,0.5497037622,0.7048173684,-0.0753523541

H,0,0.4048695426,-1.027583566,0.2412637628

H,0,-0.0038691647,-0.2217940621,4.3396069645

H,0,1.6477517776,0.4695331342,4.2268883051

H,0,0.2123923327,1.5191664239,3.9900828731

TS M062X 23PSPCMDMSO

/home/biswas/TSfordynamicpsTSsfordynamicsm062xb3lypd2b3lyppsandsb/TSfordyna

micps/m062x.log

Nitro TS

m062x/6-31+G**

E(RM062X) = -876.822188745

Zero-point correction= 0.275739 (Hartree/Particle)

Thermal correction to Energy= 0.292994

Thermal correction to Enthalpy= 0.293938

Thermal correction to Gibbs Free Energy= 0.230971

Sum of electronic and zero-point Energies= -876.546450

Sum of electronic and thermal Energies= -876.529195

Sum of electronic and thermal Enthalpies= -876.528251

Sum of electronic and thermal Free Energies= -876.591218

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	183.856	65.436	132.526

C	-0.151200	-0.704125	-1.509082
C	1.167904	-0.320274	-1.286025
C	1.851061	-0.873902	-0.212941
C	1.283796	-1.867142	0.612189
C	-0.013183	-2.247497	0.383613
C	-0.781899	-1.664996	-0.670919
C	-2.172734	-1.822976	-0.748352
N	-2.665397	0.097874	0.171972
C	-1.853881	1.072638	-0.290743
C	-0.630021	1.519033	0.332720
O	-0.089878	2.529132	-0.398338
C	1.167611	3.021651	0.065047
C	-2.573353	-0.307550	1.587252
C	-4.060208	0.180856	-0.304768
O	-0.100893	1.116824	1.362070
N	3.201114	-0.428089	0.057848
O	3.672864	0.473288	-0.629825
O	3.819253	-0.960516	0.973906
H	-0.682422	-0.315661	-2.371616
H	1.651888	0.416983	-1.916491

H	1.867794	-2.295509	1.417370
H	-0.477149	-2.996821	1.019155
H	-2.686563	-1.549644	-1.664761
H	-2.673287	-2.546465	-0.109945
H	-1.567628	-0.661670	1.802667
H	-3.305370	-1.095761	1.759042
H	-2.795775	0.556552	2.220250
H	-4.552722	-0.775705	-0.132327
H	-4.577389	0.973101	0.244253
H	-4.062534	0.409513	-1.370271
H	-2.145541	1.549190	-1.217301
H	1.085983	3.385632	1.091275
H	1.927407	2.235822	0.015951
H	1.429171	3.837825	-0.606444

TS B3LYP DissPSPCMDMSO

b3lyp.log

Nitro TS

ub3lyp/6-31+G**

E(UB3LYP) = -877.209158587

Zero-point correction= 0.271923 (Hartree/Particle)

Thermal correction to Energy= 0.290047

Thermal correction to Enthalpy= 0.290991

Thermal correction to Gibbs Free Energy= 0.223926

Sum of electronic and ZPE= -876.937236

Sum of electronic and thermal Energies= -876.919111

Sum of electronic and thermal Enthalpies= -876.918167

Sum of electronic and thermal Free Energies= -876.985233

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.007	66.867	141.152

C,0,1.2828845767,-0.0880037575,3.4733952125

C,0,1.2035777796,-0.1871477561,2.1001380743

C,0,-0.0544123176,-0.3199094109,1.4294424716

C,0,-1.2310976447,-0.3394435794,2.2451164087

C,0,-1.1593810697,-0.2409448591,3.6186556182

C,0,0.1003100198,-0.1180912831,4.2412759853

C,0,-0.1288204843,-0.4678849141,0.0272548978

N,0,0.1785181253,-0.0140005157,5.6617912007

O,0,1.3013303349,0.0982028,6.2007973726

O,0,-0.8775821061,-0.0388408939,6.3309327585

N,0,-0.0457644283,-2.6321867318,-0.7420578241

C,0,-0.1080055511,-2.5743810559,-2.0909377957

C,0,-1.3162562409,-2.3798766386,-2.8561393551

O,0,-1.0230869401,-2.3766891129,-4.1869392179

C,0,-2.1316839061,-2.1795873134,-5.0846751181

C,0,1.2716905984,-3.0274750429,-0.195589499

O,0,-2.4641912804,-2.2216872529,-2.4314083214

H,0,0.7507293934,-0.271115125,-0.5743638617

H,0,-1.0885500614,-0.3739785687,-0.4672783738

H,0,-2.2017792919,-0.4247521215,1.7661434563

H,0,-2.0563830973,-0.2504075527,4.2251911289

H,0,2.2394807818,0.0180710957,3.9695417891

H,0,2.1141550149,-0.1531668674,1.5096079613

H,0,0.8355042376,-2.498744894,-2.6150205248

H,0,-1.7022103124,-2.2132159941,-6.0850754404

H,0,-2.8717695731,-2.9738439372,-4.961123862

H,0,-2.6027989907,-1.2101605237,-4.9050757554

C,0,-1.1713900559,-3.1978490466,0.0378527358

H,0,-1.0140408161,-2.9657142054,1.0896707991

H,0,-2.1091157674,-2.7799535657,-0.3145122765

H,0,-1.1740233557,-4.2845713232,-0.103016634

H,0,1.3107102647,-2.7736228721,0.8625224111

H,0,1.397862857,-4.1081802861,-0.318772686

H,0,2.0631273073,-2.5032148939,-0.7304657359

TS B3LYPD2 DissPSPCMDMSO

b3lypd2.log

Nitro TS

ub3lyp/6-31+G**

E(UB3LYP) = -877.256366640

Zero-point correction= 0.271482 (Hartree/Particle)

Thermal correction to Energy= 0.289498

Thermal correction to Enthalpy= 0.290443

Thermal correction to Gibbs Free Energy= 0.223492

Sum of electronic and ZPE= -876.984885

Sum of electronic and thermal Energies= -876.966868

Sum of electronic and thermal Enthalpies= -876.965924

Sum of electronic and thermal Free Energies= -877.032875

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	181.663	66.715	140.910

C,0,1.2683027291,-0.1495916004,3.3898176304

C,0,1.2005092708,-0.2028955694,2.0128514606

C,0,-0.0535425094,-0.3047082403,1.3325672371

C,0,-1.2397981038,-0.343233022,2.1310871601

C,0,-1.1805658118,-0.2902665299,3.5079930726

C,0,0.0763709397,-0.1966231617,4.1441419964

C,0,-0.1141793801,-0.4302897155,-0.0689034782

N,0,0.1424165211,-0.1419124981,5.5702899528

O,0,1.2609078788,-0.0579432755,6.1225295964

O,0,-0.9199062082,-0.1804739409,6.2282298427

N,0,-0.0280837532,-2.5924513515,-0.6773771128

C,0,-0.0883505399,-2.6199284503,-2.0354316363

C,0,-1.2832588767,-2.3479962579,-2.788039684

O,0,-1.0327896415,-2.4552350938,-4.1244064834

C,0,-2.1445031292,-2.1791225375,-4.9979250965

C,0,1.2775415472,-2.9704988345,-0.1020737043

O,0,-2.3953075856,-2.0380424089,-2.346527964

H,0,0.779014447,-0.2588365584,-0.6587409771

H,0,-1.0698476317,-0.3588723272,-0.5763546766

H,0,-2.2028530982,-0.4150855604,1.6352300797

H,0,-2.0822785705,-0.3167400277,4.107011784

H,0,2.2206495938,-0.0696848857,3.8989104777

H,0,2.1136904164,-0.1622615842,1.4270444459

H,0,0.8579070369,-2.6323388959,-2.5607345051

H,0,-1.7612964134,-2.3223836341,-6.0087944072

H,0,-2.9682693956,-2.8703072873,-4.7962165217

H,0,-2.4907980111,-1.1504166406,-4.8593125872

C,0,-1.1551902571,-3.1086115629,0.1295327291

H,0,-0.9930137619,-2.8158523907,1.166838846

H,0,-2.0890426109,-2.6978260662,-0.2446797433

H,0,-1.1606819259,-4.2019116099,0.0480722746

H,0,1.3102800301,-2.6391955661,0.9364766378

H,0,1.3865231251,-4.0598931704,-0.1471111215

H,0,2.0769816798,-2.4909377443,-0.6691175248

TS M062X DissPSPCMDMSO

m062x.log

Nitro TS

um062x/6-31+G**

E(UM062X) = -876.810702539

Zero-point correction= 0.274327 (Hartree/Particle)

Thermal correction to Energy= 0.292384

Thermal correction to Enthalpy= 0.293328

Thermal correction to Gibbs Free Energy= 0.226154

Sum of electronic and ZPE= -876.536376

Sum of electronic and thermal Energies= -876.518319

Sum of electronic and thermal Enthalpies= -876.517374

Sum of electronic and thermal Free Energies= -876.584549

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	183.474	66.276	141.380

C,0,1.2330509266,-0.1749723466,3.4311705136

C,0,1.2184713465,-0.2537516217,2.0554773986

C,0,-0.0075137204,-0.3244877491,1.3309931981

C,0,-1.2223866682,-0.3076816426,2.0777449677

C,0,-1.2163048649,-0.2268202635,3.4526095518

C,0,0.013709632,-0.1636300853,4.1238535084

C,0,-0.0197249766,-0.4598558244,-0.0727901548

N,0,0.023940476,-0.076010643,5.5597941268

O,0,1.1074159314,-0.0253517023,6.1389705974

O,0,-1.0516007055,-0.054954937,6.1555773516

N,0,0.0298392726,-2.6366299684,-0.7023123609

C,0,-0.0694574144,-2.6317739904,-2.0561623463

C,0,-1.2893098557,-2.3392413171,-2.7563707418

O,0,-1.1021059827,-2.4146828978,-4.0967078564

C,0,-2.246326426,-2.1161405188,-4.8976838738

C,0,1.3421239022,-3.0336083449,-0.176081985

O,0,-2.3759481521,-2.037356214,-2.2661181217

H,0,0.8972098012,-0.315524881,-0.6343752101

H,0,-0.956071739,-0.3696104453,-0.6144466264

H,0,-2.1676040967,-0.3556306037,1.5448683918

H,0,-2.1394085891,-0.2080822246,4.0190301645

H,0,2.1641989171,-0.1172996275,3.9816345706

H,0,2.1560543684,-0.2552057795,1.5069757856

H,0,0.8549784009,-2.6560280292,-2.6186439837

H,0,-1.9148551282,-2.2092305717,-5.930179308

H,0,-3.0521534811,-2.8241996945,-4.6919097274

H,0,-2.5977305786,-1.1009223632,-4.7010169313

C,0,-1.0770343615,-3.1487005761,0.1212066417

H,0,-0.8646497577,-2.9103476199,1.1638215009

H,0,-2.0127329186,-2.6930267687,-0.1902570617

H,0,-1.1298942863,-4.2362241165,-0.0022156392

H,0,1.4096905379,-2.7293863318,0.8695199683

H,0,1.4509243031,-4.1208233924,-0.2473686214

H,0,2.1287438875,-2.5451749077,-0.7517296878

TS M062X 23SBPCMDMSO Explicit MeOH

m062x3.log

Nitro TS

m062x/6-31G*

E(RM062X) = -992.449537379

Zero-point correction= 0.332478 (Hartree/Particle)

Thermal correction to Energy= 0.353763

Thermal correction to Enthalpy= 0.354707

Thermal correction to Gibbs Free Energy= 0.283459

Sum of electronic and ZPE= -992.117059

Sum of electronic and thermal Energies= -992.095775

Sum of electronic and thermal Enthalpies= -992.094831

Sum of electronic and thermal Free Energies= -992.166078

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	221.989	78.584	149.953

C,0,-1.0078351768,-0.6347802527,1.9519750992

C,0,-0.7293835284,-1.0380252017,3.2619123568

C,0,0.5469355669,-0.8668745527,3.7608806738

C,0,1.5722707012,-0.2430367682,3.009998435

C,0,1.2980673057,0.1739778756,1.7400022614

C,0,-0.0098097469,0.0178766957,1.1604599766

C,0,-0.2557972522,0.2829720628,-0.1743944247

N,0,-0.232606107,-2.049759825,-0.656919988

C,0,-0.8535290694,-2.6612522892,0.3548538421

C,0,-0.205868208,-3.315561573,1.4773349863

O,0,-1.129058832,-3.9245693926,2.2434230333

C,0,-0.6334969433,-4.5199471383,3.4431901848

C,0,1.2222105502,-2.1548488206,-0.8229949831

C,0,-0.980228965,-1.9411311099,-1.9174422948

O,0,0.9911299573,-3.3511784233,1.7323840054

N,0,0.8242775875,-1.2620459634,5.1229521572

O,0,0.0409640114,-2.0272766773,5.6807986522

O,0,1.812818999,-0.8027345932,5.6733530449

H,0,-2.0344812044,-0.6508247319,1.6009963641

H,0,-1.4964963544,-1.4872780241,3.8831180527

H,0,2.5528764806,-0.1251739658,3.4542352247

H,0,2.0740553788,0.6475806878,1.1440707008

H,0,-1.2744078446,0.3069157325,-0.5484904233

H,0,0.5096811576,0.7286586686,-0.8038753955

H,0,1.718712651,-1.8241302933,0.0876409992

H,0,1.5087160204,-1.5233575003,-1.6631322061

H,0,1.4948637303,-3.1956771842,-1.0248454174

H,0,-0.5562436896,-1.13246898,-2.5121771004

H,0,-0.9076346593,-2.8854459639,-2.4669658587

H,0,-2.0262582671,-1.723976248,-1.6997917981

H,0,-1.9272127484,-2.7727238737,0.277217065

H,0,0.1421119699,-5.2559743193,3.2150347066

H,0,-0.2342813695,-3.7486921518,4.1092362608

H,0,-1.4899769342,-5.0070099613,3.9062021182

H,0,1.9169175996,-3.4097539048,3.3399992828

O,0,2.5073926066,-3.1865239058,4.082035195

C,0,2.4239091274,-4.1874931242,5.0732487597

H,0,3.1825154565,-3.9644620547,5.8281042064

H,0,1.4451478976,-4.1972378473,5.5726893

H,0,2.6245621453,-5.1904981076,4.6731279454

TS M062X 23SBPCMDMSO

m062x.log

Alanine dimethylallyl TSfreq

m062x/6-31G*

E(RM062X) = -876.773128990

Zero-point correction= 0.278096 (Hartree/Particle)

Thermal correction to Energy= 0.295000

Thermal correction to Enthalpy= 0.295944

Thermal correction to Gibbs Free Energy= 0.234370

Sum of electronic and ZPE= -876.495033

Sum of electronic and thermal Energies= -876.478129

Sum of electronic and thermal Enthalpies= -876.477185

Sum of electronic and thermal Free Energies= -876.538759

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	185.115	64.910	129.592

C,0,-1.1413126104,-0.4897925749,1.9392729783

C,0,-1.0658654414,-0.8502708531,3.2820740556

C,0,0.1599955011,-0.7770327708,3.9220152742

C,0,1.3137481146,-0.2727879214,3.2893387659

C,0,1.2319925979,0.0928319358,1.9721440655

C,0,0.0072917471,-0.0192862125,1.2465971463

C,0,-0.0351515907,0.0684233187,-0.1511007624

N,0,-0.0619631937,-2.0741758628,-0.4979146152

C,0,-0.872245653,-2.6955014909,0.3864070555

C,0,-0.4587834117,-3.2826411751,1.6389332935

O,0,-1.540606493,-3.8279651701,2.2555607986

C,0,-1.2835125588,-4.3945279899,3.5368690787

C,0,1.3891809265,-2.3240915705,-0.4323340383

C,0,-0.5696402272,-2.0426709308,-1.8819852402

O,0,0.6586244338,-3.3375675567,2.1320253893

N,0,0.2543393942,-1.2084978544,5.3010808561

O,0,-0.7339756065,-1.7085948877,5.8282575018

O,0,1.3205367032,-1.0632614756,5.8836586937

H,0,-2.1032697347,-0.4908354064,1.4375845845

H,0,-1.9358781535,-1.2121245063,3.8177814754

H,0,2.2401321258,-0.2006373422,3.8452765663

H,0,2.1131635313,0.4665213638,1.4573672918

H,0,-0.9935400134,0.1986020292,-0.6450737845

H,0,0.8359751524,0.4188395065,-0.6993030299

H,0,1.7610953937,-2.0420378985,0.5501551994

H,0,1.8682734751,-1.7338994574,-1.2130829679

H,0,1.5756930346,-3.3893591967,-0.5973705847

H,0,-0.0107262213,-1.2976549371,-2.4483488458

H,0,-0.4429961654,-3.0307236194,-2.3340797828

H,0,-1.6269679873,-1.7772917118,-1.8694941128

H,0,-1.921707394,-2.7462944601,0.1295625027

H,0,-0.4849378082,-5.1373849233,3.4805757207

H,0,-1.0025389492,-3.6167612257,4.2536864061

H,0,-2.2161339181,-4.8655621718,3.8454520645

TS M062X 23PSPCMDMSO Explicit MeOH

m062x3.log

Nitro TS

m062x/6-31+G**

E(RM062X) = -992.512822191

Zero-point correction= 0.329947 (Hartree/Particle)

Thermal correction to Energy= 0.351480

Thermal correction to Enthalpy= 0.352425

Thermal correction to Gibbs Free Energy= 0.280329

Sum of electronic and ZPE= -992.182875

Sum of electronic and thermal Energies= -992.161342

Sum of electronic and thermal Enthalpies= -992.160398

Sum of electronic and thermal Free Energies= -992.232493

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	220.557	79.179	151.739

C,0,-1.0271509391,-0.6003839828,1.9893948926

C,0,-0.7252057584,-0.9953616932,3.2922774208

C,0,0.5586264751,-0.7978519031,3.7749865466

C,0,1.5632412642,-0.165290477,3.0062598977

C,0,1.2683639914,0.2233785844,1.7287162676

C,0,-0.040519261,0.028974033,1.1675016328

C,0,-0.3013103113,0.2459103516,-0.178968539

N,0,-0.2131148041,-2.0590938334,-0.6515271395

C,0,-0.8488414696,-2.7022838102,0.3314331513

C,0,-0.2251095528,-3.3168274084,1.4870923037

O,0,-1.1548627958,-3.9475864627,2.2305741304

C,0,-0.6901931517,-4.5336274894,3.4497750887

C,0,1.2482143062,-2.1475814183,-0.7910331331

C,0,-0.9306603392,-1.9625380715,-1.9340962518

O,0,0.9651969769,-3.3165458517,1.7869223144

N,0,0.8623493396,-1.189989612,5.1309631544

O,0,0.1097608066,-1.9828290483,5.6945060135

O,0,1.8496323906,-0.7080865492,5.6724176044

H,0,-2.0531809921,-0.6590344033,1.6415250682

H,0,-1.4786992257,-1.4495450897,3.92672237

H,0,2.5479004254,-0.0213737248,3.4343881292

H,0,2.0320766048,0.69384596,1.115223816

H,0,-1.3243485287,0.243868136,-0.540653098

H,0,0.4521259381,0.6882164199,-0.8249625957

H,0,1.7270443544,-1.8306599546,0.1333628158

H,0,1.5441623832,-1.5010291962,-1.6157400233

H,0,1.5288602426,-3.1835669715,-1.0062957596

H,0,-0.5076464642,-1.1444868865,-2.5156932366

H,0,-0.8182300868,-2.9050833393,-2.479352195

H,0,-1.9864718965,-1.7709016622,-1.74438062

H,0,-1.9210136585,-2.8160819351,0.2337759822

H,0,0.1154243409,-5.2445153801,3.2501324368

H,0,-0.3428075073,-3.7544691075,4.1363873331

H,0,-1.5501352708,-5.0480886823,3.8742798895

H,0,1.9480354892,-3.3531702868,3.3509175066

O,0,2.5796852389,-3.2316177199,4.0801316891

C,0,2.4332982414,-4.2688267251,5.0325626599

H,0,3.2487211818,-4.1693657688,5.752511339

H,0,1.4828756083,-4.188242055,5.5760033688

H,0,2.4994364143,-5.2619999848,4.5714027684

TS M062X DissPSPCMDMSO Explicit MeOH

m062x3diss.log

Nitro TS

um062x/6-31+G**

E(UM062X) = -992.497330771

Zero-point correction= 0.327950 (Hartree/Particle)

Thermal correction to Energy= 0.350760

Thermal correction to Enthalpy= 0.351704

Thermal correction to Gibbs Free Energy= 0.270581

Sum of electronic and ZPE= -992.169380

Sum of electronic and thermal Energies= -992.146571

Sum of electronic and thermal Enthalpies= -992.145627

Sum of electronic and thermal Free Energies= -992.226750

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 220.105 79.976 170.738

C,0,0.9454691468,-0.198832047,3.3791155438

C,0,1.0977073591,-0.3319755449,2.0153024193

C,0,-0.0250443718,-0.2911834667,1.139233965

C,0,-1.3142932638,-0.100642448,1.7161384391

C,0,-1.4745464027,0.0364425281,3.0778230539

C,0,-0.3419415783,-0.0176302651,3.9020357542

C,0,0.1258367434,-0.4868403895,-0.2502388233

N,0,-0.5061501106,0.1243537142,5.3273405034

O,0,0.4917991336,0.0689366104,6.0417113978

O,0,-1.6381574665,0.2948558945,5.7732315892

N,0,-0.0063865479,-2.7020689024,-0.7815070639

C,0,0.0401028202,-2.7549845076,-2.1387991443

C,0,-1.0452150784,-2.3451785571,-2.9739589166

O,0,-0.7581663813,-2.5182745499,-4.2824039051

C,0,-1.7743112418,-2.117918099,-5.2036718062

C,0,1.1894600667,-3.2107451591,-0.0984080672

O,0,-2.1221016157,-1.8667972797,-2.5978724685

H,0,1.1169812798,-0.4797452773,-0.6910576641

H,0,-0.7182249998,-0.3229929184,-0.9124171019

H,0,-2.1822850423,-0.0598514803,1.0641570475

H,0,-2.453134092,0.186070484,3.5175043731

H,0,1.7986796942,-0.2283053469,4.0458251976

H,0,2.0905492354,-0.4650455655,1.5952740771

H,0,1.0043877614,-2.9366017112,-2.5955073019

H,0,-1.3675545613,-2.313594377,-6.193657432

H,0,-2.6845152767,-2.7022910462,-5.0476838491

H,0,-1.9968866245,-1.0539088858,-5.0913164632

C,0,-1.2448837227,-3.0471093205,-0.065331985

H,0,-1.1151974512,-2.7864569622,0.9854937672

H,0,-2.0857610617,-2.5046202919,-0.4889201991

H,0,-1.4116687014,-4.1261695379,-0.1563903822

H,0,1.1804556042,-2.8616235679,0.9353149839

H,0,1.1826301723,-4.3057823656,-0.1122859277

H,0,2.0823806624,-2.840026106,-0.6022325538

H,0,-3.7572704443,-1.389178648,-3.2888899544

O,0,-4.7050161164,-1.1897128443,-3.3745931058

C,0,-5.3018218974,-1.4831359379,-2.1230522393

H,0,-6.3644159312,-1.2426115018,-2.1964277282

H,0,-5.2013442305,-2.5446437847,-1.8650616873

H,0,-4.8635754675,-0.8837325378,-1.3154293419